

**OPTIMAL TUNDISH DESIGN METHODOLOGY**  
**IN A**  
**CONTINUOUS CASTING PROCESS**

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## ABSTRACT

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**Title:** Optimal Tundish Design Methodology in a Continuous Casting Process  
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*The demand for higher quality steel and higher production rates in the production of steel slabs is ever increasing. These slabs are produced using a continuous casting process. The molten steel flow patterns inside the components of the caster play an important role in the quality of these products. A simple yet effective design method that yields optimum designs is required to design the systems influencing the flow patterns in the caster. The tundish is one of these systems. Traditionally, experimental methods were used in the design of these tundishes, making use of plant trials or water modelling. These methods are both costly and time consuming. More recently, Computational Fluid Dynamics (CFD) has established itself as a viable alternative to reduce the number of experimentation required, resulting in a reduction in the time scales and cost of the design process. Furthermore, CFD provides more insight into the flow process that is not available through experimentation only. The CFD process is usually based on a trial-and-error basis and relies heavily on the insight and experience of the designer to improve designs. Even an experienced designer will only be able to improve the design and does not necessarily guarantee optimum results. In this thesis, a more efficient design methodology is proposed. This methodology involves the combination of a mathematical optimiser with CFD to automate the design process. The methodology is tested on a four different industrial test cases. The first case involves the optimisation of a simple dam-weir configuration of a single strand caster. The position of the dam and weir relative to inlet region is optimised to reduce the dead volume and increase the inclusion removal. The second*

*case involves the optimisation of a pouring box and baffle of a two-strand caster. In this case, the pouring box and baffle geometry is optimised to maximise the minimum residence time at operating level and a typical transition level. The third case deals with the geometry optimisation of an impact pad to reduce the surface turbulence that should result in a reduction in the particle entrainment from the slag layer. The last case continues from the third case where a dam position and height is optimised in conjunction with the optimised impact pad to maximise the inclusion removal on the slag layer. The cases studies show that a mathematical optimiser combined with CFD is a superior alternative compared to traditional design methods, in that it yields optimum designs for a tundish in a continuous casting system.*

**Keywords:** *tundish, continuous casting, computational fluid dynamics, mathematical optimisation, computational flow optimisation, design methodology, steelmaking, inclusion removal, tundish design*

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## SAMEVATTING

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**Titel:** Optimale Gietbak Ontwerpsmetodiek van 'n Kontinue-gietproses  
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*Daar bestaan 'n alomtoenemende aanvraag vir hoër kwaliteit staalplate wat teen 'n hoër tempo geproduseer word. Die plate word geproduseer deur 'n kontinue gietproses. Die vloeistaal patrone in die proses speel 'n belangrike rol in die kwaliteit van die produkte. 'n Eenvoudige maar tog effektiewe ontwerpsmetode word verlang wat optimum ontwerp lewer van die sisteme wat die vloeipatrone beïnvloed. Die gietbak is een van die sisteme. Histories is eksperimentele metodes gebruik in die ontwerp van die gietbakke, met gebruikmaking van aanlegtoetse of water modellering. Meer onlangs is Berekenings Vloei Dinamika (BVD) gebruik as 'n alternatief om die aantal eksperimentele toetse te verminder en om sodoende die tydskaal en kostes van die ontwerpsproses te verminder. Verder verskaf BVD baie meer insig in die vloei proses wat nie beskikbaar is met tradisionele eksperimentele metodes nie. Die BVD proses is gewoonlik gebaseer op 'n tref-of-fouteer basis en steun sterk op die ontwerper se insig en ondervinding om die ontwerp te verbeter. Selfs 'n ontwerper met baie ondervinding sal slegs die ontwerp kan verbeter en sal nie noodwendig 'n optimum ontwerp kan gee nie. In die tesis word 'n meer effektiewe ontwerpsmetodiek voorgestel. Die metodiek behels die kombinerings van 'n wiskundige optimerings program met BVD om die ontwerpsproses te outomatiseer. Die metodiek word getoets op vier verskillende toetsgevalle. Die eerste geval is die optimering van 'n eenvoudige dam-keermuur konfigurasie vir 'n enkelstring gietproses. Die posisie van die dam en keermuur relatief tot die inlaat area is geoptimeer om die dooie volume verminder en die inklusie verwydering te vermeerder. Die tweede geval beskryf die optimering van die gietboks en skermplaat van 'n tweestring gietbak. In die geval*

*word die gietboks en skermplaat geometrie geoptimeer om die minimum residensie tyd te maksimeer by die bedryfsvlak en by 'n tipiese transisievlak. Die derde geval beskou die geometrie optimering van 'n impakstuk om die oppervlak turbulensie te verlaag, wat veroorsaak dat minder partikels in die vloei ingetrek sal word vanaf die slaklaag. Die laaste geval volg op geval drie waar 'n dam se posisie en hoogte geoptimeer word saam met die geoptimeerde impakstuk om die inklusie verwydering op die slaklaag te maksimeer. Die toetsgevalle wys dat 'n wiskundige optimeerder gekombineerd met BVD 'n beter alternatief is as tradisionele ontwerpmetodes, om sodoende optimum ontwerpe van 'n gietbak van 'n kontinue stringgiet proses te lewer.*

**Sleutelwoorde:** *gietbak, stringgiet, berekenings vloei dinamika, wiskundige optimering, berekenings vloei optimering, ontwerpmetodiek, staalmaak, inklusieverwydering, gietbak ontwerp*

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## NOMENCLATURE

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**Symbols:**

<b>Variable</b>	<b>Description</b>	<b>Unit</b>
$a_1, a_2, a_3$	Constants for particle drag law	-
$A$	Approximated Hessian matrix	-
$a$	Approximated curvature	-
$C_D$	Particle drag coefficient	-
$C_L$	Constant for eddy lifetime	-
$C_\mu$	Empirical constant for $k$ - $\varepsilon$ turbulence model	-
$C_1$	Empirical constant for $k$ - $\varepsilon$ turbulence model	-
$C_2$	Empirical constant for $k$ - $\varepsilon$ turbulence model	-
$c_p$	Specific heat at constant pressure	J/kg·K
$D_{eff}$	Local effective diffusion coefficient	m <sup>2</sup> /s
$D_0$	Laminar diffusion coefficient	m <sup>2</sup> /s
$D/Dt$	Substantial derivative	-
$d_p$	Particle diameter	M
$E$	Empirical constant for the wall function in turbulent flow	-
$f$	Objective function	♦
Fr	Froude number	-
$g$	Gravitational acceleration	m/s <sup>2</sup>
$g_j$	$j$ -th inequality constraint	♦
$H$	Fluid enthalpy	J/kg
H	Hessian matrix	-
$h_k$	$k$ -th inequality constraint	♦
$I$	Identity matrix	-
$K$	Thermal conductivity	W/m·K

---

♦ Problem dependant

Variable	Description	Unit
$k$	Turbulent kinetic energy	$\text{m}^2/\text{s}^2$
$k_P$	Turbulent kinetic energy at point $P$	$\text{m}^2/\text{s}^2$
$L$	Reference length	m
	Turbulent length scale	m
$L_e$	Eddy length scale	m
$m$	Number of inequality constraints	-
$n$	Number of design variables	-
$\bar{p}$	Time-averaged pressure equations	Pa
$p$	Pressure	Pa
	Penalty function	-
	Number of equality constraints	-
Re	Reynolds Number	-
$Sc_t$	Turbulent Schmitt number	-
$S_m$	Mass source	$\text{kg}/\text{m}^3 \cdot \text{s}$
$t$	Time	s
$t_{cross}$	Particle eddy crossing time	s
$T$	Temperature	K
$T_0$	Reference temperature	K
$U$	Reference velocity	m/s
$u$	Velocity in $x$ -direction	m/s
$U^*$	Dimensionless velocity	-
$u_i$	Instantaneous velocity in the $i$ -th direction	m/s
$U_i$	Mean velocity in the $i$ -th direction	m/s
$u_i'$	Fluctuating part of velocity in the $i$ -th direction	m/s
$U_P$	Mean velocity of the fluid at point $P$	m/s
$u_p$	Particle velocity	m/s
$\bar{\mathbf{V}}$	Time-averaged velocity vector	m/s
$\mathbf{V}$	Velocity vector	m/s
$v$	Velocity in $y$ -direction	m/s
$V_{dpv}$	Dispersed plug volume	-
$V_{dv}$	Dead volume	-
$V_{mv}$	Well-mixed volume	-



Variable	Description	Unit
$V_{pv}$	Plug flow volume	-
$\nu_t$	Eddy viscosity	$\text{m}^2/\text{s}$
$w$	Velocity in $z$ -direction	$\text{m}/\text{s}$
$x$	Distance in $x$ -direction	$\text{m}$
$\mathbf{x}$	Design variable vector	♦
$\mathbf{x}^*$	Optimum design variable vector	♦
$x_i$	Spatial co-ordinate in the $i$ -direction	$\text{m}$
	$i$ -th design variable	♦
$y$	Distance in $y$ -direction	$\text{m}$
$Y$	Inclusion mass fraction	-
$y^*$	Dimensionless distance fro the wall	-
$y_P$	Distance from point $P$ to the wall	$\text{m}$
$z$	Distance in $z$ -direction	$\text{m}$
$\alpha$	Penalty function parameter for inequality constraint	-
$\beta$	Thermal expansion coefficient	$1/\text{K}$
	Penalty function parameter for equality constraint	-
$\gamma$	Penalty function parameter for objective function	-
$\delta_i$	Move limit on $i$ -th design variable	♦
$\delta_{ij}$	Kronecker delta function	-
$\varepsilon$	Turbulent dissipation rate	$\text{m}^2/\text{s}^3$
$\zeta$	Normally distributed random number	-
$\theta_{av}$	Average residence time	-
$\theta_{min}$	Minimum break-through time	-
$\theta_{peak}$	Time to reach peak concentration	-
$\kappa$	Von Kármán constant	-
$\lambda$	Bulk viscosity	$\text{m}/\text{s}^2$
$\mu$	Kinematic viscosity	$\text{m}^2/\text{s}$
	Large positive number	-
$\rho$	Density	$\text{kg}/\text{m}^3$
	Penalty function parameter	-

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♦ Problem dependant

Variable	Description	Unit
$\rho_0$	Reference density	kg/m <sup>3</sup>
$\rho_p$	Particle density	kg/m <sup>3</sup>
$\sigma_\varepsilon$	Empirical constant for $k$ - $\varepsilon$ turbulence model	-
$\sigma_k$	Empirical constant for $k$ - $\varepsilon$ turbulence model	-
$\tau$	Theoretical residence time	-
	Particle relaxation time	-
$\tau_e$	Characteristic lifetime of an eddy	s
$\omega$	Turbulent vorticity	1/s
$\Delta x_{\text{norm}}$	Normalized step size	-
$\Delta f_{\text{norm}}$	normalized change in function value	-
$\Delta x_i$	Step size for $i$ -th design variable	♦
$\Phi$	Viscous dissipation	W/m <sup>3</sup>

**Abbreviations:**

CFD	Computational Fluid Dynamics
RANS	Reynolds Averaged Navier-Stokes equation
RTD	Residence time distribution
MRT	Minimum residence time
RSM	Reynolds Stress Models
ASM	Algebraic Stress Models
LES	Large-Eddy Simulation
DNS	Direct Numerical Simulation
SEN	Submerged Entry Nozzle

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♦ Problem dependant

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## CHAPTER 1: INTRODUCTION

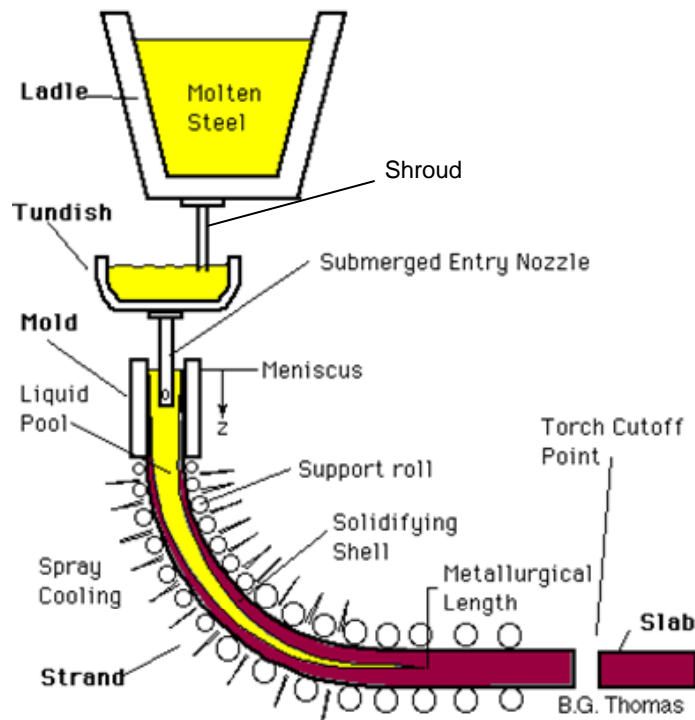
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### 1-1 BACKGROUND

The continuous casting of metals is not a very old process in the manufacturing process. The continuous strip casting process was conceived by Henry Bessemer in 1858 but only became widespread in the 1960s [1]. The continuous casting process however increased significantly since then and now, most basic metals are mass-produced using a continuous casting process. In 1992, continuous casting was used to produce over 90% of steel in the world, including carbon, alloy and stainless steel grades [2]. In 2001 over 500 million tons of steel, 20 million tons of aluminium and 1 million tons of copper, nickel and other metals were produced in a continuous casting process [1]. It is estimated that the total world production of crude steel will increase to over 900 million tons per year in 2010 with steel produced by continuous casting still making up 90% of this production [2].

A graphic representation of the continuous casting process is given in Figure 1-1 [3]. This figure shows the different entities of the continuous casting process. These entities are:

- the ladle and shroud,
- the tundish,
- the submerged entry nozzle (SEN) and mould and
- the solidifying strand and slab.



**Figure 1-1: Schematic representation of the continuous casting process [3]**

The continuous casting process will now be briefly described [4]. Scrap metal and ore are melted in a furnace (typically either in a basic oxygen furnace or an electric arc furnace) upstream of the continuous caster. The steel is then poured from the furnace into a ladle where it undergoes different metallurgical processes before it reaches the continuous caster, i.e., excess oxygen is removed from the molten steel in a vacuum degasser, and second-metallurgy stations ensure the correct composition of the steel. The steel is shielded from the air by using a slag cover on top of the molten steel.

The ladle is then brought to the continuous caster where the steel is poured from the ladle through a ceramic nozzle called the shroud into the tundish. The shroud is used to shield the steel from the air when steel flows from the ladle to the tundish. A control valve at the outlet of the ladle controls the flow rate into tundish. The liquid steel is again shielded from the air by a slag layer to prevent oxidation that would form detrimental oxide inclusions in the steel.

The molten steel flows through the tundish and exits the tundish through the submerged entry nozzle (SEN) into a bottomless mould. The walls of the mould,

usually made of copper, are water-cooled, which causes the steel to solidify on the sides. The sides of the mould are usually oscillating to prevent “sticking” of the steel to the sides of the mould.

Drive rollers lower in the casting machine continuously withdraw the solidifying shell from the mould. The speed of the rollers is set so that the material exiting the mould matches that of the incoming flow into the tundish so that the caster runs in steady state most of the time. Water jets sprayed on the strand, as it exits the mould, cools the strand further, causing the solidifying shell to grow to the core of the strand. The supporting rollers hold the strand in place as the core of the strand solidifies. The core of the strand continues to solidify for a significant length after exiting the mould. The point where the whole slab is fully solidified can be in the order of tenths of meters downstream of the mould.

The solidified strand at the end of the rollers is then cut into slabs by a torch. These slabs are then processed further, e.g., the slabs are hot and cold rolled into sheets, bars, rails and other shapes.

Because of the nature of the continuous casting process, the tundish has traditionally acted purely as a reservoir when one ladle is emptied and when a new ladle is brought into place. In the last couple of decades, the role of the tundish in the continuous casting process has evolved from that of a reservoir between the ladle and mould to being a grade separator, an inclusion removal device and a metallurgical reactor. For both grade separation and inclusion removal, the flow patterns inside the tundish play an important role. For the former, the flow patterns determine the amount of mixing that occurs, while for the latter, the paths of inclusion particles are influenced by the flow field. Several tundish designs and tundish devices or furniture exist that have as their aim the modification of tundish flow patterns, to either minimize mixed-grade length during transition, and/or to increase inclusion particle removal by the slag layer.

At the initiation of this study, steel producing plants in South Africa are experiencing difficulties with more economical and higher quality steel production in the

continuous casting process. Tons of steel are downgraded or scrapped at continuous casting plants. The typical difficulties of these plants are:

- downgrading or scrapping of steel due to inclusions and slag entrainment in the ladle, tundish and mould,
- downgrading or scrapping of mixed-grade sections during grade transitions,
- downgrading or scrapping of first section of new cast,
- break-outs of the strand,
- nozzle clogging due to solidifying steel,
- low yield levels in the tundish when draining the tundish at the end of a sequence due to slag entrainment and vortex formation.

## **1-2 EXISTING KNOWLEDGE**

Tundish design is traditionally performed through experimental plant trials or water modelling. For the former, due to the nature of the process, it is difficult to have an exact knowledge of the flow field. Indirect measurements such as copper traces and oxygen sensing give an indication of the residence time and inclusion particles present in the tundish. Water modelling on the other hand, provided that Reynolds number and Froude number similarity for steady-state conditions can be achieved [5,6,7,8], can provide more insight into the mixing characteristics. In order to include thermal effects however, water models require significant modification to address cases where buoyancy effects and natural convection plays a measurable role [9,10].

With the advent of powerful computers and fluid flow modelling software, Computational Fluid Dynamics (CFD) has become an alternative tool with which to assess different tundish designs [11,12,13,14]. Not only can the thermal effects be incorporated, but also every detail of the flow field becomes available for extracting measures of performance.

### **1-3 RESEARCH OBJECTIVES**

The objectives of this study are to:

- develop a methodology for the design optimisation of tundish and tundish furniture,
- apply the methodology to the design of specific products used in the tundish in the South African continuous casting industry.

### **1-4 SCOPE OF THE STUDY**

In this study, the focus is placed on the design of a tundish and the tundish furniture to improve the molten steel flow patterns. The method developed in this study will be applied to a single strand caster of Columbus Stainless Steel as well as the two strand continuous caster of ISCOR Vanderbijlpark. The optimisation methodology can however be extended to other areas of the continuous casting process as well as other fluid flow and heat transfer applications where CFD is used to analyse the design.

CFD as analysis tool only, has limitations in that the variation of many parameters require trial-and-error simulations of which the interpretation relies heavily on the insight of the modeller. This usually leads to non-optimal solutions and furthermore requires a lot of manual labour by the engineer doing the modelling. In this study, a more efficient method is developed which combines CFD with mathematical optimisation. This means that the design parameters become design variables and that the performance trends with respect to these variables are taken into account automatically by the optimisation algorithm. Using this method, an optimum design for the tundish and its furniture can be found.

### **1-5 ORGANISATION OF THE THESIS**

The thesis consists of the following chapters:

- Chapter 2 gives the appropriate literature pertaining the modelling of tundishes and optimisation tools. This chapter describes the relevant theory behind physical modelling and numerical modelling of tundishes. The chapter also

gives the theory of two mathematical optimisation methods that will be used in the rest of the study.

- Chapter 3 then develops the methodology for optimising tundish furniture. This chapter looks at the different important aspects in the tundish and tundish furniture design using a mathematical optimisation method. The different steps involved in a mathematical optimisation study is given and it is shown how an optimisation method links with a commercial CFD code.
- Chapter 4 applies this methodology to four different case studies. The methodology developed in Chapter 3 is applied to these case studies to show that the optimisation methodology is a viable alternative in the design of tundish and tundish furniture.
- Chapter 5 gives the conclusions drawn from this study.
- Chapter 6 give recommendations and possibility of future research in this field.



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## CHAPTER 2: LITERATURE STUDY

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### 2-1 INTRODUCTION

This chapter gives the literature pertaining to this thesis. The literature study is divided into two main parts. The first part is on the modelling and design of the tundish and tundish furniture. The second part provides a background to mathematical optimisation. The modelling and design section is divided into three main parts, i.e., physical modelling, plant trials and numerical modelling. The mathematical optimisation section describes the theory behind mathematical optimisation and a description of the different optimisers used in this thesis.

### 2-2 TUNDISH MODELLING AND DESIGN

#### ***2-2.1 The Continuous Casting Process***

In the last couple of decades, the role of the tundish in the continuous casting process has evolved from that of a reservoir between the ladle and mould to being a grade separator, an inclusion removal device and a metallurgical reactor. For both grade separation and inclusion removal, the flow patterns inside the tundish play an important role. For the former, the flow patterns determine the amount of mixing that occurs, while for the latter, the paths of inclusion particles are influenced by the flow field. Several tundish designs and tundish devices or furniture exist that have as their aim the modification of tundish flow patterns, to either minimise mixed-grade length during transition, and/or to increase inclusion particle removal by the slag layer.

The modelling and design of the tundish and tundish furniture can be divided into three main categories, i.e., physical modelling, plant trials and mathematical modelling. These three categories will now be described in more detail.

### **2-2.2 Physical Modelling**

Physical modelling has great benefits over doing plant trials, i.e.:

- It does not operate under such harsh environments under which the tundish operates in the plant (e.g., extreme high temperatures and almost no visual observations possible).
- It does not interfere with the production of the plant.
- It can be a lot more repeatable due to the more stringent control one has in the laboratory whereas in the plant there are other variables that cannot be controlled.

Most modelling is done using water as the fluid representing the liquid steel. This is due to the similarity of the kinematic viscosity of molten steel at typical temperatures inside the tundish and water at room temperature as shown in Table 2-1 [15].

**Table 2-1: Physical properties of water at 20°C and steel at 1600°C [15]**

	Water (20°C)	Steel (1600°C)
Molecular viscosity [kg/m·s]	0.001	0.0064
Density [kg/m <sup>3</sup> ]	1 000	7014
Kinematic viscosity [m <sup>2</sup> /s]	1×10 <sup>-6</sup>	0.913×10 <sup>-6</sup>
Surface tension [N/m]	0.073	1.6

In reduced scale isothermal studies, dynamic and geometric similarities must be obeyed. Geometric similarity simply implies that every dimension in the scale model bears a fixed ratio to corresponding dimension in the full scale.

Dynamic similarity implies that the ratio of the different forces acting on a small fluid element must be the same in the scale model and in the full-scale version [16].

Considering dynamic similarity, the inertial, viscous and gravitational forces are of importance in tundish flows. These forces are characterised by two dimensionless numbers. The first is the Reynolds  $\left( Re = \frac{\rho UL}{\mu} \right)$  number that gives the ratio of the inertia forces to the viscous forces. The second is the Froude number  $\left( Fr = \frac{U^2}{gL} \right)$  that gives the ratio of the inertia forces to gravitational forces. When water at room temperature is used as the modelling fluid, matching of both Reynolds and Froude numbers is only possible using full-scale models. In reduced-scale models, either Reynolds or Froude numbers can be satisfied, but not both [17].

Full scale, as well as reduced scale, water modelling has been performed extensively [5,14,18,19,20]. In order to include thermal effects however, water models require significant modification to address cases where buoyancy effects and natural convection plays a measurable role [10, 21]. This makes the use of numerical modelling as discussed later, an attractive alternative.

To quantify the performance of the tundish, two different types of approaches have been commonly applied by researchers [16]:

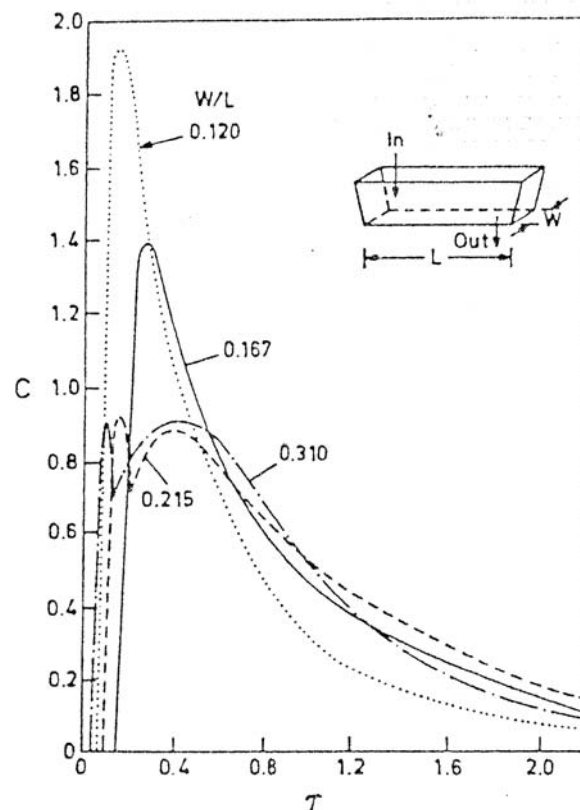
1. the measurement of residence time distribution (RTD)
2. direct measurement of inclusion separation through aqueous simulation.

The residence time of fluid within a reactor is defined as the time a single fluid element spends in the reactor vessel. The theoretical residence time is defined as:

$$\tau \equiv \frac{\text{Filled Volume of the tundish}}{\text{Volumetric flow rate of steel into the tundish}} \quad (2-1)$$

Usually flow in any tundish is accompanied by a distribution of residence times for different fluid elements (i.e., some fluid elements stay longer while others spend shorter times within the tundish with respect to the theoretical residence time) [16]. These residence time distributions can be experimentally measured by injecting a tracer (pulse or continuous) at the inlet of the tundish and then dynamically measuring the concentration at the outlet using colourimetry, conductimetry, or spectrophotometry.

When injecting a pulse injection at time  $t = 0$ , a typical concentration profile at the outlet, also called the C curve [22], is obtained as shown in Figure 2-1 [23]. Typical C curves or Residence Time Distribution (RTD) for different dimensionless tundish widths are shown in this figure.



**Figure 2-1: Typical measured RTD curve in a water model of a single strand slab casting tundish system at various values of the dimensionless tundish width [23]**

From a typical RTD curve, different performance-related criteria for the tundish can be extracted. The values of the minimum break-through time ( $\theta_{\min}$  in dimensionless form), time to attain the peak concentration ( $\theta_{peak}$ ), and the average residence time ( $\theta_{av}$ ) can be incorporated into an appropriate flow model to estimate the proportions of dead ( $V_{dv}$ ), plug ( $V_{pv}$ ), and well-mixed volumes ( $V_{mv}$ ). The minimum break through time is also referenced to as the Minimum Residence Time (MRT). Kemeny *et al.* [15] proposed the various fractional volumes as:

$$\begin{aligned} V_{dv} &= 1 - \theta_{av} \\ V_{pv} &= \theta_{\min} = \theta_{peak} \\ V_{mv} &= \frac{1}{C_{peak}} \end{aligned} \quad (2-2)$$

As pointed out by Sahai and Ahuja [6] this model has two shortcomings:

1. Considerable axial or longitudinal diffusion is present in tundish systems, causing the minimum break-through time and the time to reach the peak concentration not to be equal.
2. The three volume fractions do not add up to unity, which is a requirement for the mixed model.

Sahai and Ahuja [6] proposed a modified mixed model for tundish systems. Instead of dividing the tundish into a dead volume, plug-flow volume and well-mixed volume, they defined a dead volume, dispersed plug-flow volume ( $V_{dpv}$ ) and a well-mixed volume as follows:

$$\begin{aligned} V_{dv} &= 1 - \theta_{av} \\ V_{dpv} &= \frac{(\theta_{\min} + \theta_{peak})}{2} \\ V_{mv} &= 1 - V_{dv} - V_{dpv} \end{aligned} \quad (2-3)$$

Several investigators have also carried out direct measurement of particle removal in water models [24,25,26]. In these studies, hollow glass spheres were introduced into the tundish via the shroud. The exit particle

concentration was monitored with various techniques. Nakajama *et al.* [24] showed that any increase in the plug flow volume leads to an increase in the separation efficiency. This type of measurements however needs considerable hardware upgrades to an existing water model.

### **2-2.3 Plant Trials**

The high temperature associated with the continuous casting process makes it very difficult to do on-site plant trials. Typical plant operations take a few discrete temperature measurements at regular intervals. Some tundishes have been instrumented to give on-line tundish wall temperatures [27]

A RTD curve can also be constructed by doing a copper trace trial. A copper dosage is introduced near the shroud of the tundish. Samples are then taken from the mould at regular intervals. These samples are then analysed for the copper concentration using a photo-spectrometer [28]. The principle of the analysis method is optical emission spectroscopy [29]. The sample material is vaporised by an arc. The atoms and ions contained in the atomic vapour are excited into emission of radiation. The radiation emitted is passed to the spectrometer optics via an optical fibre, where it is dispersed into its spectral components. From the range of wavelengths emitted by each element, the composition of the steel can be determined.

The last common practice to be used in plant trials is taking samples at the shroud and SEN to determine the number of inclusions present in the steel. Many measurement techniques exist to evaluate the steel cleanliness as given by Zhang *et al* [30]. The steel cleanliness at the shroud and SEN are then compared to each other to determine the efficiency of tundish in terms of particle removal.

As mentioned earlier, there are two major drawbacks of doing plant trials. Firstly, it interferes with production of the plant. Secondly, due to a large number of other uncontrollable parameters on the plant, the trials are

unrepeatable and therefore it is difficult to isolate the influence of certain parameters on the performance of the tundish.

### **2-2.4 Numerical Modelling**

Computational Fluid Dynamics (CFD) is a numerical modelling technique that solves the Navier-Stokes equations on a discretised domain of the geometry of interest with the appropriate flow boundary conditions supplied. The Navier-Stokes equations are a complex non-linear set of partial differential equations that describes the mass and momentum conservation of a fluid. Additional physics can also be resolved by solving additional conservation equations, e.g., heat transfer, multi-phase flow, and combustion. A CFD analysis consists of the following steps [31]:

- Problem Identification and Pre-Processing
  - Define your modelling goals
  - Identify the domain you will model
  - Design and create the grid
- Solver Execution
  - Set up the numerical model
  - Compute and monitor the solution
- Post-Processing
  - Examine the results
  - Consider revisions to the model

Some of these steps will now be discussed in more detail.

#### **2-2.4.1 Grid Generation**

The grid generation process deals with the division of the domain under consideration into small control volumes on which the discretised governing equations will be solved.

The grid generation forms a large part in terms of person-hour time of the CFD analysis. A large amount of time has gone into and is currently going into the development of commercial automated grid

generators. Once such product is GAMBIT (Geometry and Mesh Building Intelligent Toolkit) [32]. GAMBIT uses solid modelling techniques to create a virtual model of the geometry under consideration. Various grid generation tools are available to create a grid in this geometry. The grid generation tools are available to create hexahedron, tetrahedron, prism and pyramid cells.

GAMBIT makes use of a Graphical User Interface (GUI) where the user is able to give commands to manipulate and generate the grid via the input of values and appropriate mouse clicks. An important aspect of GAMBIT with respect to mathematical optimisation is the parameterisation and automation of the set-up of the model and grid generation using journal files. A journal file is a text file that contains text commands that give the instructions to GAMBIT to generate a model without the use of the GUI.

#### **2-2.4.2 Conservation Equations**

The governing equations that describe the flow field are a set of non-linear partial differential equations. The equations are derived from mass, momentum and energy conservation. These three different governing equations will now be discussed briefly.

##### Conservation of Mass

The conservation of mass in Eulerian terms in its most common general form for fluids is given in the following [33]:

$$\frac{\partial \rho}{\partial t} + \text{div} \rho \mathbf{V} = S_m \quad (2-4)$$

where  $\rho$  is the density,  $t$  is the time,  $\mathbf{V}$  is the velocity vector of the fluid and  $S_m$  is a mass source. For a constant density, equation (2-4) simply reduces to the following:

$$\text{div} \mathbf{V} = 0 \quad (2-5)$$

The constant density assumption can be made for tundishes when the temperature differences are not too large. The effect of the buoyancy



of the higher temperature steel is then treated through the Boussinesq model in the momentum transport equation. More detail on this model is given below.

### Transport of Momentum

The Navier-Stokes equations are derived from the conservation of momentum (Newton's second law). The set of equations can be written in Eulerian terms as a single vector equation using the indicial notation [33]:

$$\rho \frac{D\mathbf{V}}{Dt} = \rho \mathbf{g} - \nabla p + \frac{\partial}{\partial x_j} \left[ \mu \left( \frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} \right) + \delta_{ij} \lambda \operatorname{div} \mathbf{V} \right] \quad (2-6)$$

where  $\mathbf{g}$  is the gravitation vector,  $x_i$  is the spatial co-ordinate,  $v_i$  is the  $i$ -component of the velocity vector,  $\mu$  is the ordinary coefficient of viscosity,  $\lambda$  is the coefficient of bulk viscosity,  $\delta_{ij}$  is the Kronecker delta function ( $\delta_{ij}=1$  if  $i=j$  and  $\delta_{ij}=0$  if  $i \neq j$ ) and  $\frac{D}{Dt}$  the total or substantial derivative. The relation between the ordinary viscosity and bulk viscosity is given by Stokes' hypothesis [34]:

$$\lambda + \frac{2}{3} \mu = 0 \quad (2-7)$$

As an example, equation (2-6) is written out in full for the  $i$ -direction in the following equation:

$$\begin{aligned} \rho \frac{Du}{Dt} = \rho g_x - \frac{\partial p}{\partial x} + \frac{\partial}{\partial x} \left( 2\mu \frac{\partial u}{\partial x} + \lambda \operatorname{div} \mathbf{V} \right) + \frac{\partial}{\partial y} \left[ \mu \left( \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) \right] \\ + \frac{\partial}{\partial z} \left[ \mu \left( \frac{\partial u}{\partial z} + \frac{\partial w}{\partial x} \right) \right] \end{aligned} \quad (2-8)$$

When assuming incompressible flow with a constant viscosity, equation (2-6) reduces considerably to the following:

$$\rho \frac{D\mathbf{V}}{Dt} = \rho \mathbf{g} - \nabla p + \mu \nabla^2 \mathbf{V} \quad (2-9)$$

For many natural-convection flows, you can get faster convergence with the Boussinesq model (originally published in [35] as cited in [36]) than you can get by setting up the problem with fluid density as a function of temperature. This model treats density as a constant value in all solved equations, except for a momentum source term in the momentum equation:

$$(\rho - \rho_0)g \approx -\rho_0\beta(T - T_0)g \quad (2-10)$$

where  $\rho_0$  is the (constant) density of the fluid,  $T_0$  is the operating temperature, and  $\beta$  is the thermal expansion coefficient. Equation (2-10) is obtained by using the Boussinesq approximation  $\rho = \rho_0(1 - \beta\Delta T)$  to eliminate  $\rho$  from the buoyancy term. This approximation is accurate as long as changes in actual density are small; specifically, the Boussinesq approximation is valid when  $\beta(T - T_0) \ll 1$  [37]. The term on the left of this equation ( $\beta(T - T_0)$ ) is the fraction of the change in density relative to the reference density, implying that the change in density should be small relative to the reference density.

### Transport of Energy

The energy equation is derived from the first law of thermodynamics. The energy relation in Eulerian terms is given by the following if it is assumed that the conduction heat fluxes are given by Fourier's Law and that radiative effects are negligible [33]:

$$\rho \frac{Dh}{Dt} = \frac{Dp}{Dt} + \text{div}(k\nabla T) + \Phi \quad (2-11)$$

where  $h$  is the fluid enthalpy,  $k$  is the thermal conductivity,  $T$  is the temperature of the fluid and  $\Phi$  is the viscous dissipation and is given by:

$$\Phi = \mu \left[ 2 \left( \frac{\partial u}{\partial x} \right)^2 + 2 \left( \frac{\partial v}{\partial y} \right)^2 + 2 \left( \frac{\partial w}{\partial z} \right)^2 + \left( \frac{\partial v}{\partial x} + \frac{\partial u}{\partial y} \right)^2 + \left( \frac{\partial w}{\partial y} + \frac{\partial v}{\partial z} \right)^2 + \left( \frac{\partial u}{\partial z} + \frac{\partial w}{\partial x} \right)^2 \right] + \lambda \left( \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \right)^2 \quad (2-12)$$

Again assuming incompressible flow as well as a constant thermal conductivity and low-velocity flow where the viscous-dissipation ( $\Phi$ ) is zero, equation (2-11) reduces considerably to the following:

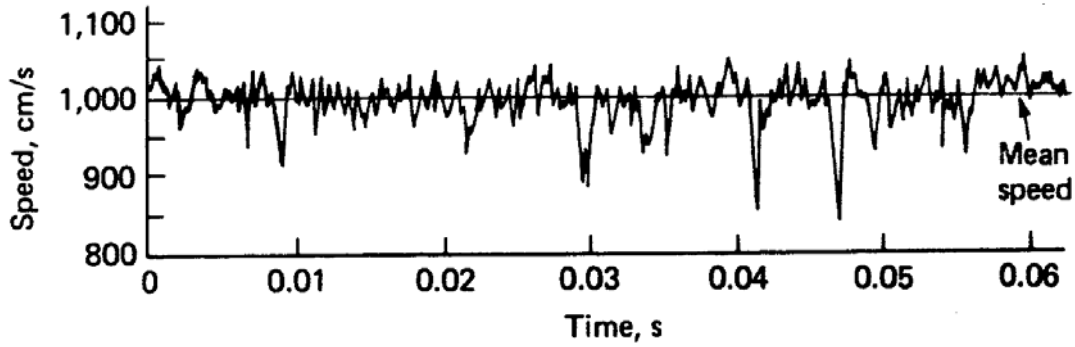
$$\rho c_p \frac{DT}{Dt} = k \nabla^2 T \quad (2-13)$$

### **2-2.4.3 Turbulence Modelling**

Turbulence models are used in CFD because of the fact that the small-scale fluctuations of the flow field cannot be resolved when solving the above-mentioned governing equations on an ordinary grid. Instead, the ensemble average of the basic conservation equations is taken to give the Reynolds-Averaged Navier-Stokes (RANS) formulation. The RANS formulation is derived from the assumption that every solved for quantity consists of a mean part as given and a fluctuating part. For instance, the  $u_i$  velocity component is decomposed into a mean part and a fluctuating part as given in equation (2-14).

$$u_i(\vec{x}, t) = U_i(\vec{x}, t) + u_i'(\vec{x}, t) \quad (2-14)$$

Figure 2-2 shows a typical behaviour for the  $u_i$  velocity component but all the flow quantities that are solved for are assumed to be of a similar form.



**Figure 2-2: Typical time variation of the  $u_i$ -velocity component in a flow field [33]**

By substituting the assumed decomposition of the solved for quantities as given in (2-14) into the Navier-Stokes and simplifying, we get the RANS equations. For example, the RANS formulation for the momentum equation for incompressible flow with constant viscosity is given in equation (2-15) [33].

$$\rho \frac{D\bar{\mathbf{V}}}{Dt} + \rho \frac{\partial}{\partial x_j} (\overline{u'_i u'_j}) = \rho \mathbf{g} - \nabla \bar{p} + \mu \nabla^2 \bar{\mathbf{V}} \quad (2-15)$$

where  $u'_i$  are the small fluctuations in the velocity of the flow field, and  $\bar{\mathbf{V}}$  and  $\bar{p}$  indicate the time-averaged velocity vector and pressure respectively.

Comparing equation (2-9) and equation (2-15) it can be seen that the momentum equation is complicated by an extra term called the turbulent inertia tensor or Reynolds stresses  $(\overline{u'_i u'_j})$ . This term's analytical form is not known beforehand. This symmetrical inertia tensor introduces six new variables in 3-D, which can only be calculated through a detailed knowledge of the turbulent structure. This turbulent structure is however unknown at the start of a calculation. The effect of the small-scale fluctuations is therefore rather represented by a turbulence model than calculating the turbulent inertia tensor. The available turbulence models can be divided into the following groups.

### Zero-equation models

These models are simple algebraic models and are computationally inexpensive. The accuracy obtained with these types of models is sometimes not sufficient especially in very complex flow, due to the fact that no information from the surrounding flow field is used. Some examples of these types of turbulence models are the mixing-length model and the Baldwin-Lomax model [38].

### One-equation models

One-equation turbulence models model the turbulent kinetic energy ( $k$ ) equation. These models satisfy the transport of the turbulent kinetic energy. The turbulent length scales in these models are correlated with algebraic equations [39]. The results obtained with these types of models are satisfactory but no better than the zero-equation models resulting in the fact that these models are not very popular. An exception is the Spallart-Almaras model that has been developed for high speed external flow applications.

### Two-equation models

In two-equation turbulence models, a second equation is coupled with the turbulent kinetic energy equation used in the one-equation models. The second equation models for example the rate of change of either dissipation ( $\varepsilon$ ), turbulent length scale ( $L$ ) or vorticity ( $\omega$ ).

The most popular scheme is probably the standard  $k$ - $\varepsilon$  model [40,41,42] or some derivative of it like the renormalisation group (RNG)  $k$ - $\varepsilon$  model [43]. This model is also used throughout this study. The two equations that describe the turbulent kinetic energy ( $k$ ) and turbulent dissipation ( $\varepsilon$ ) are given in the following two equations.

$$\frac{Dk}{Dt} = \frac{\partial}{\partial x_j} \left( \frac{v_t}{\sigma_k} \frac{\partial k}{\partial x_j} \right) + v_t \frac{\partial \bar{u}_i}{\partial x_j} \left( \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) - \varepsilon \quad (2-16)$$

$$\frac{D\varepsilon}{Dt} = \frac{\partial}{\partial x_j} \left( \frac{v_t}{\sigma_\varepsilon} \frac{\partial \varepsilon}{\partial x_j} \right) + C_1 v_t \frac{\varepsilon}{k} \frac{\partial \bar{u}_i}{\partial x_j} \left( \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) - C_2 \frac{\varepsilon^2}{k} \quad (2-17)$$

where  $\sigma_k$ ,  $\sigma_\varepsilon$ ,  $C_1$  and  $C_2$  are empirical constants and  $v_t$  is the eddy viscosity. The eddy viscosity is modelled as follows:

$$v_t = \frac{\mu_t}{\rho} = \frac{C_\mu k^2}{\varepsilon} \quad (2-18)$$

where  $C_\mu$  is an empirical constant.

The recommended values for the empirical constants are [33]:

$$C_\mu = 0.09 \quad C_1 = 1.44 \quad C_2 = 1.92 \quad \sigma_k = 1.0 \quad \sigma_\varepsilon = 1.3 \quad (2-19)$$

These values are not universal and have to be modified for other type of flows, e.g., recirculating flows.

#### Wall-function approach

Equations (2-16) and (2-17) are not valid near a boundary wall because sublayer damping effects are neglected in the model. Wall functions are therefore used near the wall. The use of wall functions also avoids the need for a very fine grid near the wall. An example of wall functions as proposed by Launder and Spalding's law of the wall [40,44] is:

$$U^* = \frac{1}{\kappa} \ln(Ey^*)$$

$$\text{with } U^* = \frac{U_P C_\mu^{1/4} k_P^{1/2}}{\tau_w / \rho} \quad (2-20)$$

$$\text{and } y^* = \frac{\rho C_\mu^{1/4} k_P^{1/2} y_P}{\mu}$$

where  $\kappa$  is the Von Kármán constant (= 0.42),  $E$  an empirical constant (= 9.81),  $U_P$  the mean velocity of the fluid at point  $P$ ,  $k_P$  the turbulent

kinetic energy at point  $P$ ,  $y_P$  the distance from point  $P$  to the wall, and  $\mu$  the dynamic viscosity of the fluid.

The effect of turbulence in all the above-mentioned models is modelled as an increase in the viscosity. This is called the eddy-viscosity concept. The dynamic viscosity ( $\mu$ ) used in equations (2-6) and (2-12) is the total viscosity and is expressed as the sum of the molecular viscosity of the fluid plus the turbulent viscosity ( $\mu_t$ ). The turbulent viscosity is directly calculated from the turbulent kinetic energy and turbulent dissipation rate. For the standard  $k$ - $\varepsilon$  model this relationship is given in equation (2-18).

#### Other Methods

Another approach in turbulence modelling is to model the Reynolds stresses  $(-\rho \overline{u_i u_j})$  using partial differential equations [45]. These are called the Reynolds Stress Models (RSM). The RSM model is at a level higher than the previous schemes and therefore provides second-order turbulent closure at the cost of computational complexity. Another method to reduce the complexity of the RSM approach, is to model the Reynolds stresses by a purely algebraic equation with the same characteristics than the differential equations [46]. These methods are called the Algebraic Stress Models (ASM). Both these Reynolds stress models, RSM and ASM, have the potential for greater accuracy, mainly because the turbulence in the flow is not assumed to be isotropic as the previous methods (i.e., the zero-, one and two-equation models).

Currently a lot of research is conducted on Large-Eddy Simulation (LES) in which only the smallest fluctuations (or sub-grid scales) are modelled using a simple turbulence model (e.g.,  $k$ - $\varepsilon$  turbulence model). Modelling the turbulence in this way requires an unsteady simulation with a very fine grid distribution, making this model computational

very expensive. For industrial applications, like the tundish, this model is computationally too expensive.

Currently another active research topic is that of Direct Numerical Simulation (DNS). This method for calculating turbulent flow is direct in that it does not use turbulence models. Consequently, a very fine grid and small time step are required. The method is even more computationally expensive than the LES model. This method is currently considered as the state-of-the-art method for turbulent flow calculations but is restricted to very simple flow cases with a low Reynolds number making it impractical for industrial applications of CFD.

#### **2-2.4.4 Inclusion modelling**

Modelling of the non-metallic inclusion in steel melt can be done in a number of ways [47]. The different methods will now be briefly discussed.

##### Lagrangian particle tracking

The trajectory of a discrete phase particle (or inclusion) can be predicted by integrating the force balance on the particle, which is written in a Lagrangian reference frame. This force balance equates the particle inertia with the forces acting on the particle, and can be written (for the  $x$ -direction in Cartesian coordinates) as [37]:

$$\frac{du_p}{dt} = F_D(u - u_p) + \frac{g_x(\rho_p - \rho)}{\rho_p} + F_x \quad (2-21)$$

where  $F_D(u - u_p)$  is the drag force per unit particle mass and

$$F_D = \frac{18\mu}{\rho_p d_p^2} \frac{C_D \text{Re}}{24} \quad (2-22)$$

Here,  $u$  is the fluid phase velocity,  $u_p$  is the particle velocity,  $\mu$  is the molecular viscosity of the fluid,  $\rho$  is the fluid density,  $\rho_p$  is the density



of the particle, and  $d_p$  is the particle diameter.  $Re$  is the relative Reynolds number, which is defined as

$$Re = \frac{\rho d_p |u_p - u|}{\mu} \quad (2-23)$$

The drag coefficient,  $C_D$ , is taken from:

$$C_D = a_1 + \frac{a_2}{Re} + \frac{a_3}{Re^2} \quad (2-24)$$

where  $a_1$ ,  $a_2$ , and  $a_3$  are constants that apply for smooth spherical particles over several ranges of Reynolds number given by Morsi and Alexander [48].

The effect of a turbulent flow field in the above-mentioned method does not include the effect of turbulence on the particle trajectory. One approach to include the effect of turbulence is through stochastic tracking. This approach predicts the turbulent dispersion of particles by integrating the trajectory equations for individual particles, using the instantaneous fluid velocity, e.g., for the  $x$ -direction  $\bar{u} + u'(t)$ , along the particle path during the integration. By computing the trajectory in this manner for a sufficient number of representative particles, the random effects of turbulence on the particle dispersion may be accounted for [37]. The velocity fluctuations that prevail during the lifetime of the turbulent eddy are sampled by assuming that they obey a Gaussian probability distribution. This results in the fluctuation velocity in the  $x$ -direction to be:

$$u' = \zeta \sqrt{u'^2} \quad (2-25)$$

where  $\zeta$  is a normally distributed random number and  $\sqrt{u'^2}$  is the local RMS value of the velocity fluctuations. Since the kinetic energy of turbulence is known at each point in the flow (from the appropriate turbulence model), these values of the RMS fluctuating components can be obtained (assuming isotropy) as:

$$\sqrt{u'^2} = \sqrt{\frac{2k}{3}} \quad (2-26)$$

The characteristic lifetime of the eddy is best calculated by assuming a random variation about  $T_L$  :

$$\tau_e = -T_L \log(r) \quad (2-27)$$

where  $r$  is a uniform random number between 0 and 1,  $T_L$  is given by  $C_L \frac{k}{\varepsilon}$  with  $C_L \approx 0.15$  when used in conjunction with the  $k$ - $\varepsilon$  turbulence model [49].

The particle eddy crossing time is defined as

$$t_{cross} = -\tau \ln \left[ 1 - \left( \frac{L_e}{\tau |u - u_p|} \right) \right] \quad (2-28)$$

where  $\tau$  is the particle relaxation time,  $L_e$  is the eddy length scale, and  $|u - u_p|$  is the magnitude of the relative velocity.

The particle is assumed to interact with the fluid phase eddy over the smaller of the eddy lifetime and the eddy crossing time. When this time is reached, a new value of the instantaneous velocity is obtained by applying a new value of  $\zeta$  in (2-25) [31].

#### Inclusion diffusion model

The second method makes use of a species diffusion model to calculate the distribution of small inclusions [47]. This method solves the convection-diffusion equation of a species inside the tundish as given in equation (2-29) to give the time evolution of the inclusion mass fraction,  $Y$ :

$$\frac{\partial}{\partial t}(\rho Y) + \frac{\partial}{\partial x_i}(\rho u_i Y) + \frac{\partial}{\partial x_i} \left( \rho D_{eff} \frac{\partial Y}{\partial x_i} \right) = 0 \quad (2-29)$$

where  $D_{eff}$  is the local effective diffusion coefficient and is dependent on the local turbulence and dissipation levels as calculated from the turbulence model as given in (2-30):

$$D_{eff} = D_0 + \frac{\mu_t}{\rho Sc_t} \quad (2-30)$$

where  $D_0$  is the laminar diffusion coefficient and  $Sc_t$  is the turbulent Schmidt number.

The flotation of inclusions, reoxidation, and collision agglomeration are ignored in this model which is only used to investigate general transient mixing behaviour.

#### Lumped inclusion removal model with size function

The last model calculates the evolution of the inclusion size distribution for the duration of its residence time in the tundish (developed by Miki *et al* [50]). This model considers the collision of particles due to both turbulence and differences in flotation removal rate of each inclusion size. This is a lumped model based on uniform average properties within the tundish. The collision rate due to turbulent eddy motion is governed by the mean turbulent dissipation level,  $\varepsilon$ , and the cluster size of the inclusion. Details of this model can be found in [47,50].

#### **2-2.4.5 Solution Algorithm**

The finite volume approach as implemented in the commercial CFD solver, FLUENT [37] is used in this study. In this method, the governing equations are first integrated on the individual control volumes that were created in the grid generation phase, to construct algebraic equations for the discrete dependent variables such as velocities, pressure, temperature, and conserved scalars. Secondly, the

discretised equations are linearised and the resulting linear equation system is solved to yield updated values of the dependent variables.

In this study, the segregated solution method of FLUENT is used. In this approach, the governing equations are solved sequentially (i.e., segregated from one another). Because the governing equations are non-linear (and coupled), several iterations of the solution loop must be performed before a converged solution is obtained. Each iteration consists of the steps illustrated in Figure 2-3 and outlined below [37]:

- Fluid properties are updated, based on the current solution. (If the calculation has just begun, the fluid properties will be updated based on the initialised solution.)
- The  $u$ ,  $v$  and  $w$  momentum equations are each solved in turn using current values for pressure and face mass fluxes, in order to update the velocity field.
- Since the velocities obtained in the previous step may not satisfy the continuity equation locally, a ‘Poisson-type’ equation for the pressure correction is derived from the continuity equation and the linearised momentum equations. This pressure correction equation is then solved to obtain the necessary corrections to the pressure and velocity fields and face mass fluxes such that continuity is satisfied.
- Equations for scalars such as turbulence, energy and species are solved using the previously updated values of the other variables.
- A check for convergence of the equation set is made.

These steps are continued until the convergence criteria are met.

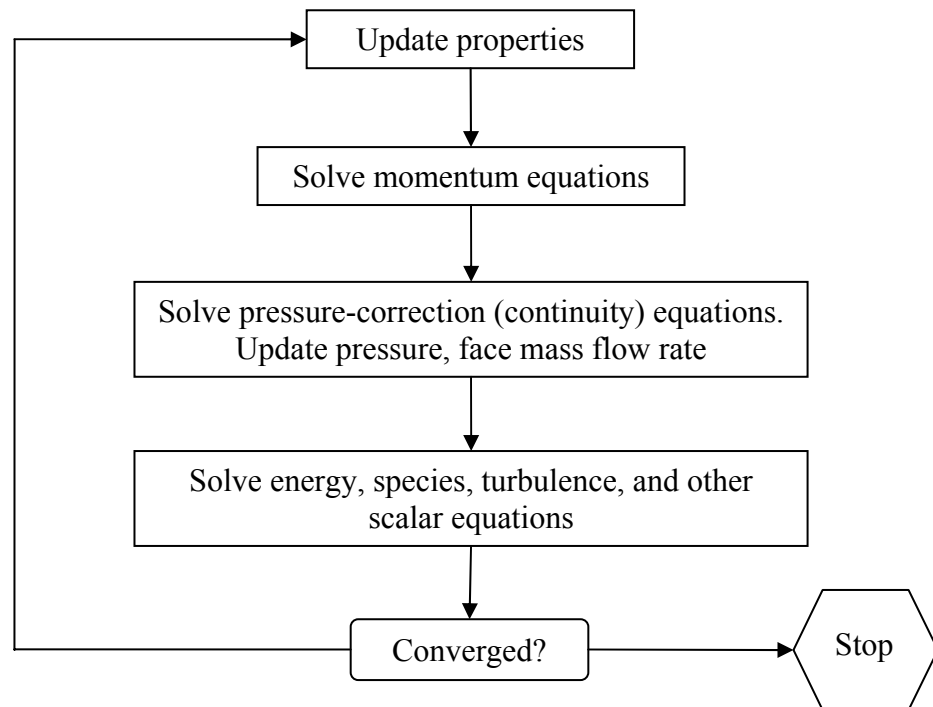


Figure 2-3: Overview of the Segregated Solution Method [37]

## 2-3 MATHEMATICAL OPTIMISATION

### 2-3.1 Definition of Mathematical Optimisation

Mathematical optimisation can be described as the systematic approach to find the minimum (or maximum) of a specific function given a set of constraints. In an engineering application, this relates to the case of finding the best design under certain design constraints by changing the appropriate design variables.

### 2-3.2 The Non-Linear Optimisation Problem

The non-linear constrained optimisation problem can be defined in general in the following standard way:

$$\min_{\mathbf{x}} f(\mathbf{x}); \quad \mathbf{x} = [x_1, x_2, \dots, x_i, \dots, x_n]^T, \quad x_i \in R$$

$$\text{Subject to: } \begin{aligned} g_j(\mathbf{x}) &\leq 0; & j &= 1, 2, \dots, m \\ h_k(\mathbf{x}) &= 0; & k &= 1, 2, \dots, p < n \end{aligned} \quad (2-31)$$

where  $f(\mathbf{x})$ ,  $g_j(\mathbf{x})$  and  $h_k(\mathbf{x})$  are scalar functions of the vector  $\mathbf{x}$ .

The function  $f(\mathbf{x})$  is the objective function (or sometimes called the cost function) that is being minimised. The functions  $g_j(\mathbf{x})$  and  $h_k(\mathbf{x})$  are the inequality and equality constraints respectively. The variable  $n$  is called the dimension of the optimisation problem. The components of the vector  $\mathbf{x}$  are called the design variables. The solution to problem (2-31) is given by the vector  $\mathbf{x}^*$ :

$$\mathbf{x}^* = [x_1^*; x_2^*; \dots; x_n^*]^T \quad (2-32)$$

and gives the lowest value for  $f(\mathbf{x})$  subject to the specified inequality and equality constraints. The solution  $\mathbf{x}^*$  may however be non-unique.

If there are no equality or inequality constraints, the optimisation problem becomes an unconstrained optimisation problem. The unconstrained optimisation problem can be more easily solved because the optimisation simply consists of finding the minimum of  $f(\mathbf{x})$ . For a constrained optimisation problem, the optimisation becomes much more complex and the constraints have to be treated in some sort of special way. The most popular way to treat these constraints is by introducing a penalty function, as will be described in the following paragraphs.

A large number of algorithms have been developed to solve the optimisation problem given in equation (2-31). Some of the state-of-the-art methods include multiplier methods and sequential quadratic programming [51, 52]. This chapter will only discuss the optimisation algorithms that were used in this study. The choice of these specific algorithms is guided the way in which each algorithm is suited for problems with computationally expensive function evaluations as well as the robustness of the algorithms. The success of the choices becomes evident in the rest of this study.

### **2-3.3 Optimisation Algorithms**

Two optimisation algorithms are investigated in this study. The first is a gradient-based optimisation algorithm of Snyman called DYNAMIC-Q, while

the second is the Successive Response Surface Method (SRSM) algorithm incorporated into the commercial optimisation program LS-OPT. Both these optimisation algorithms make use internally of another optimisation algorithm, the Leap Frog Optimisation Program (LFOPC), to optimise an approximation to the original optimisation problem. DYNAMIC-Q, SRSM and LFOPC will now be discussed in detail.

### **2-3.3.1 Snyman's Leap-Frog Optimisation Program (LFOP) Adapted to Handle Constrained Optimisation Problems (LFOPC)**

The original LFOP of Snyman [53,54] was subsequently adapted to handle constrained optimisation problems [55,56,57]. This is achieved by applying the original LFOP to a penalty function formulation of the original problem. The appropriate penalty function formulation is given in equation (2-33).

$$p(\mathbf{x}) = \gamma f(\mathbf{x}) + \sum_{j=1}^m \alpha_j g_j^2(\mathbf{x}) + \sum_{k=1}^p \beta_k h_k^2(\mathbf{x}) \quad (2-33)$$

where  $\alpha_j = \begin{cases} 0 & \text{if } g_j(\mathbf{x}) \leq 0 \\ \rho_j & \text{if } g_j(\mathbf{x}) > 0 \end{cases}$ ,  $\rho_j$  and  $\beta_k$  are large positive numbers

and  $\gamma = 1$  (unless otherwise stated).

For simplicity, the penalty parameters,  $\rho_j, j = 1, 2, \dots, m$  and  $\beta_k, k = 1, 2, \dots, p$  take on the same positive value,  $\rho_j = \beta_k = \mu$ . The unconstrained minimum of  $p(\mathbf{x})$  tends to the constrained minimum of problem (2-31) as  $\mu$  tends to infinity. The choice of  $\mu$  has received a lot of attention. For  $\mu$  very large, high accuracy is obtained, although the unconstrained minimisation problem can become ill-conditioned. For this reason, the penalty is usually increased gradually, thereby allowing a controlled approach to the solution with limited violation of the inequality constraints in the initial design steps.

The LFOPC applies the LFOP algorithm to the penalty function formulation (as given in (2-33)) in three phases. The three phases are executed in the following way [57]:

Phase 0:

In the first phase, the penalty parameter is introduced at a moderately low value. The penalty function is then minimised using the LFOP. In this phase, the value of  $\mu$  is set to  $\mu_0=10^2$ . This initial value of  $\mu$  was used throughout this study. This is possible because the LFOP automatically scales the constraints ensuring that the spatial violation of a constraint on the penalty function gradient is approximately the same for all the constraints. On convergence, this gives an approximate optimum point. The active inequality constraints are then identified. An active inequality constraint is one that is violated. In the standard formulation (2-31), this implies that the particular inequality constraint  $g_j$  is greater than or equal to zero. If no active inequality constraints are found and there are no equality constraints, the algorithm is terminated and the minimum is found. The minimum of the constrained problem in (2-31) is then the same as the minimum of the unconstrained problem. If the computational time of the optimisation program becomes significant, the following phase is sometimes skipped if the number of active constraint plus the number of equality constraint are equal to the number of design variables. The computational time associated with CFD is however, a few orders larger than the computational time of the optimisation program and therefore the following phase has never been skipped in this study.

Phase 1:

In this phase, the penalty parameter is increased. Here a value of  $\mu = 10^4$  is used. The LFOP is again used to minimise the penalty function but using the approximate design point from Phase 0 as a starting point. On convergence, a more accurate approximate solution point of the original problem given in (2-31) is found. The active set



of inequality constraints is again identified. This set might not be identical to the set identified in Phase 0.

Phase 2:

In the last phase, the LFOP is used to minimise the penalty function, again using the approximate solution of the previous phase as the starting point but with  $\gamma$  set to zero in the penalty function. This implies that LFOP seeks a solution to the intersection of the active constraints. The constrained minimum of the optimisation problem is at the minimum of the intersection of the active constraints. If the active constraints do not intersect, this algorithm will find the best possible solution by giving a compromised solution. The compromised solution usually violates the active constraints by a small amount. This ability to obtain a compromised solution makes LFOPC a very robust algorithm as will be shown in the optimisation cases investigated in the following chapters.

The dynamic trajectory method described above is applied to a sequence of approximate subproblems until convergence is obtained. The subproblems are constructed due to the fact that is very computationally expensive to evaluate the penalty function due to the required CFD simulations. If the subproblems are not constructed, the function value will have to be evaluated at each iteration of the LFOPC algorithm. Successive subproblems are constructed at relatively high computational cost, but these subproblems are solved economically using the LFOPC algorithm. The construction of the approximate subproblems is described below.

### **2-3.3.2 Snyman's DYNAMIC-Q Method**

In a complex problem where the objective function is unknown and/or is computationally expensive, the successive approximation scheme developed by Snyman *et al* [55,58,59,60] is used. This approach involves the application of the above-mentioned dynamic trajectory

method for unconstrained optimisation adapted to handle constrained problems through penalty formulations as follows. The DYNAMIC method is applied to successive approximate Quadratic subproblems of the original problem, hence the name, DYNAMIC-Q. The successive subproblems are constructed by sampling at relatively high computational expense, the behaviour of the optimisation problem at successive approximate solution points in the design space. These subproblems are approximated using the quadratic approximation of a function as discussed in the following paragraph. These subproblems, which are analytically simple, are solved quickly and economically using the LFOPC discussed above.

Successive quadratic subproblems,  $P[l]:l=1,2,\dots$ , are formed at successive design points  $\mathbf{x}^{(l)}$ . Spherically quadratic approximations are used to approximate the objective function and/or constraints, if these functions are not analytically known or computationally expensive. The approximation of the subproblems will be discussed in detail in the following paragraph.

These spherical quadratic subproblems have favourable characteristics for the optimisation program, e.g., the quadratic subproblem is smooth with no discontinuities and the subproblem usually has only one global optimum.

The application of the DYNAMIC-Q method requires the use of move limits. This is an added feature used to control convergence of the optimisation process. Essentially, it implies the placing of additional constraints that limit the movement of each of the design variables from one design point to the next design point. This is helpful in the initial steps of the optimisation run when the spherical quadratic approximation may have a large error. This implies that the next design point is not allowed to move too far from the current design point.

The move limits are implemented as additional inequality constraints in the following way:

$$\begin{aligned} x_i - x_i^{(l)} - \delta_i &\leq 0 \\ -x_i + x_i^{(l)} - \delta_i &\leq 0 \end{aligned}; \quad i = 1, 2, \dots, n \quad (2-34)$$

where in general the  $\delta_i$  are different move limits for each design variable and  $x_i^{(l)}$  is the design variable at the current design point.

The DYNAMIC-Q method has the potential to be applied to any engineering optimisation problem in which the numerical simulation is computationally expensive. The only two requirements are that the engineer has confidence in the answer obtained by the numerical analysis and that the engineer can define his/her problem as an optimisation problem. This study will apply the DYNAMIC-Q algorithm to CFD.

#### Constructing the Successive Approximate Spherical Quadratic Subproblems

The spherical quadratic approximation of a function is used in this study to approximate the functions that are not analytically known and/or computationally expensive to evaluate, to construct the subproblem at design iteration  $l$ . These functions may be the objective function or one of the constraints, depending on the optimisation problem investigated. By approximating these computationally expensive functions, the computational time is drastically reduced because only a few function evaluations are necessary to obtain the approximation. The way these successive subproblems are constructed will now be discussed in detail [55,58].

The Taylor expansion of a function  $f(\mathbf{x})$  in the region of the current design point  $\mathbf{x}^{(l)}$  is given by:

$$f(\mathbf{x}) = f(\mathbf{x}^{(l)}) + \nabla^T f(\mathbf{x}^{(l)})(\mathbf{x} - \mathbf{x}^{(l)}) + \frac{1}{2}(\mathbf{x} - \mathbf{x}^{(l)})^T \mathbf{H}(\mathbf{x}^{(l)})(\mathbf{x} - \mathbf{x}^{(l)}) + \text{H.O.T} \quad (2-35)$$

where  $\mathbf{H}(\mathbf{x}^{(l)})$  is the Hessian matrix at point  $\mathbf{x}^{(l)}$  and H.O.T are the higher order terms in the expansion. The vector  $\mathbf{x}^{(l)}$  is the current design point. The Hessian matrix is defined in equation (2-36).

$$\mathbf{H}(\mathbf{x}) = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_n} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2^2} & \cdots & \frac{\partial^2 f}{\partial x_2 \partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_n \partial x_1} & \frac{\partial^2 f}{\partial x_n \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_n^2} \end{bmatrix} (\mathbf{x}) = \nabla^2 f(\mathbf{x}) \quad (2-36)$$

Note the symmetry of this matrix because  $\frac{\partial^2 f}{\partial x_i \partial x_j} = \frac{\partial^2 f}{\partial x_j \partial x_i}$ .

If the higher order terms are ignored, the value of  $f$  at a point  $\mathbf{x}$  in the region of  $\mathbf{x}^{(l)}$  is given approximately by:

$$f(\mathbf{x}) \approx f(\mathbf{x}^{(l)}) + \nabla^T f(\mathbf{x}^{(l)})(\mathbf{x} - \mathbf{x}^{(l)}) + \frac{1}{2}(\mathbf{x} - \mathbf{x}^{(l)})^T \mathbf{H}(\mathbf{x}^{(l)})(\mathbf{x} - \mathbf{x}^{(l)}) \quad (2-37)$$

The gradient vector  $\nabla f(\mathbf{x}^{(l)})$  in equation (2-37), is approximated using a first-order forward differencing scheme. This first-order gradient approximation needs some special consideration and will be discussed in the following paragraphs.

Because the function  $f$ , or its derivatives, is not analytically known, the second-order derivatives need also to be calculated using a finite-difference approximation, e.g., a forward-differencing scheme. Furthermore, if the calculation of the function is computationally expensive to evaluate (as is the case with CFD), the calculation of the Hessian matrix becomes extremely expensive computationally. The Hessian matrix is therefore approximated. The way the Hessian matrix is approximated now follows.

Taking  $\mathbf{A}^{(l)}$  as the approximation of the Hessian matrix, the approximation  $\tilde{f}(\mathbf{x})$  to the function,  $f(\mathbf{x})$  is given by:

$$\tilde{f}(\mathbf{x}) = f(\mathbf{x}^{(l)}) + \nabla^T f(\mathbf{x}^{(l)}) (\mathbf{x} - \mathbf{x}^{(l)}) + \frac{1}{2} (\mathbf{x} - \mathbf{x}^{(l)})^T \mathbf{A}^{(l)} (\mathbf{x} - \mathbf{x}^{(l)}) \quad (2-38)$$

where the approximation of the Hessian matrix ( $\mathbf{A}^{(l)}$ ) is given by

$$\mathbf{A}^{(l)} = \text{diag}(a^{(l)}, a^{(l)}, \dots, a^{(l)}) = a^{(l)} \mathbf{I} \quad (2-39)$$

and  $\mathbf{I}$  is the identity matrix.

The appropriate constant  $a^{(l)}$  used in the construction of the approximate Hessian matrix is calculated by using function and gradient information at the design point  $\mathbf{x}^{(l)}$  and at a previous design point, say at point  $\mathbf{x}^{(l-1)}$ . The value of  $a^{(l)}$  defines the amount of curvature of the spherical quadratic approximation. During an optimisation run the point  $\mathbf{x}^{(l-1)}$  is the previous design point where the gradient and function values of the function are already known. The initial value,  $a^{(1)}$ , depends on the specific optimisation problem being considered. In this study, a value of zero was chosen for the construction of the first subproblem. This implies that the first approximation has no curvature.

If it is specified that  $\tilde{f}(\mathbf{x})$  interpolates  $f(\mathbf{x})$  at  $\mathbf{x}^{(l)}$  and  $\mathbf{x}^{(l-1)}$  and that the gradient of  $\tilde{f}(\mathbf{x})$  matches that of  $f(\mathbf{x})$  at  $\mathbf{x}^{(l)}$ , equation (2-38) can be rewritten to give  $a^{(l)}$  as follows:

$$a^{(l)} = \frac{2\{f(\mathbf{x}^{(l-1)}) - f(\mathbf{x}^{(l)}) - \nabla^T f(\mathbf{x}^{(l)}) (\mathbf{x}^{(l-1)} - \mathbf{x}^{(l)})\}}{\|\mathbf{x}^{(l)} - \mathbf{x}^{(l-1)}\|^2} \quad (2-40)$$

This may be called the backward interpolating spherical approximation to  $f(\mathbf{x})$  at  $\mathbf{x}^{(l)}$ .

Another way to calculate  $a^{(l)}$  is to specify that  $\tilde{f}(\mathbf{x})$  interpolates  $f(\mathbf{x})$  at  $\mathbf{x}^{(l)}$  and  $\mathbf{x}^{(l-1)}$  and that the gradient of  $\tilde{f}(\mathbf{x})$  matches that of  $f(\mathbf{x})$  at  $\mathbf{x}^{(l-1)}$  and not at  $\mathbf{x}^{(l)}$  as above. This may be called the forward interpolating spherical approximation. This gives an expression for  $a^{(l)}$  as follows:

$$a^{(l)} = \frac{2\{f(\mathbf{x}^{(l)}) - f(\mathbf{x}^{(l-1)}) - \nabla^T f(\mathbf{x}^{(l-1)}) (\mathbf{x}^{(l)} - \mathbf{x}^{(l-1)})\}}{\|\mathbf{x}^{(l)} - \mathbf{x}^{(l-1)}\|^2} \quad (2-41)$$

By averaging the curvature of the backward interpolating quadratic function as in (2-40), and forward interpolating quadratic approximation as in (2-41), an averaged expression for  $a^{(l)}$  can be obtained [61] and is given in (2-42).

$$a^{(l)} = \frac{(\nabla^T f(\mathbf{x}^{(l-1)}) - \nabla^T f(\mathbf{x}^{(l)})) (\mathbf{x}^{(l-1)} - \mathbf{x}^{(l)})}{\|\mathbf{x}^{(l)} - \mathbf{x}^{(l-1)}\|^2} \quad (2-42)$$

Expression (2-42) may be called the backward-forward interpolating spherical approximation and gives more stable values for the curvature. In the following chapters, it will be shown that this results in smoother convergence of the optimisation run. It must be noted that constructing  $\tilde{f}(\mathbf{x})$  using the averaged value of  $a^{(l)}$  means that it no longer necessarily interpolates  $f(\mathbf{x})$  at point  $\mathbf{x}^{(l-1)}$ .

The DYNAMIC-Q method is terminated when either the normalized step size

$$\Delta x_{\text{norm}} = \frac{\|\mathbf{x}^{(l)} - \mathbf{x}^{(l-1)}\|}{1 + \|\mathbf{x}^{(l)}\|} \quad (2-43)$$

or if the normalized change in function value

$$\Delta f_{\text{norm}} = \frac{|f^{(l)} - f_{\text{best}}|}{1 + |f_{\text{best}}|} \quad (2-44)$$

are below specified tolerances. The DYNAMIC-Q method does not guarantee a global minimum and typically, a multi-start approach (i.e. starting the optimizer from different starting designs) should be used to ensure that a global optimum is obtained.

### **2-3.3.3 Successive Response Surface Method (SRSM)**

The last optimisation method used is the Successive Response Surface Method (SRSM) [62] as implemented in LS-OPT [63]. LS-OPT is a commercial package available as part of the LS-DYNA software suite. This algorithm uses a Response Surface Methodology (RSM) [64], i.e., a meta-modelling or surrogate technique, to construct linear response surfaces on a subregion from a *D*-optimal subset of experiments. The *D*-optimality criterion is implemented using a genetic algorithm and a 50% over-sampling is typically used. Successive subproblems are solved using a multi-start variant of the Leap-Frog dynamic trajectory method of Snyman [57]. The multi-start locations are selected as the subset of experimental designs, and the best optimum is selected as the optimum of the subproblem. The size of successive subregions is adapted based on contraction and panning parameters designed to prevent oscillation and premature termination [62]. Infeasibility is handled automatically when it occurs through the construction and solution of an auxiliary problem to bring the design within the subregion if possible. As the optimum is approached, the subregion is contracted automatically, implying that inaccuracies in the sensitivity information do not cause large departures from the previous design. Therefore, this handling of the step-size dilemma also provides an inherent move limit to the algorithm.

### **2-3.4 Gradient Approximation of Objective and Constraint Functions**

The Dynamic-Q method of Snyman needs first-order gradients of the objective and constraint functions with respect to each of the design variables. There are different methods available when calculating these gradients. These different methods have certain advantages and disadvantages when using CFD to construct the gradient, as explained in the next section.

Forward-Differencing Scheme

A forward-differencing scheme is used to approximate the gradient vector of the objective function ( $\nabla f(\mathbf{x}^{(l)})$ ) when the function is approximated using the spherical quadratic approximation discussed in 2-3.3.2. The first-order gradients are calculated as follows:

$$\frac{\partial f(\mathbf{x})}{\partial x_i} = \frac{f(\mathbf{x} + \Delta \mathbf{x}_i) - f(\mathbf{x})}{\Delta x_i} \quad i = 1, 2, \dots, n \quad (2-45)$$

where

$$\Delta \mathbf{x}_i = [0, 0, \dots, \Delta x_i, \dots, 0]^T$$

The first-order gradients of the inequality and equality constraints, when these constraints are approximated using the spherical quadratic approximation, are approximated in a similar fashion and are given in (2-46).

$$\begin{aligned} \frac{\partial g_j(\mathbf{x})}{\partial x_i} &= \frac{g_j(\mathbf{x} + \Delta \mathbf{x}_i) - g_j(\mathbf{x})}{\Delta x_i} & j = 1, \dots, m \\ \frac{\partial h_k(\mathbf{x})}{\partial x_i} &= \frac{h_k(\mathbf{x} + \Delta \mathbf{x}_i) - h_k(\mathbf{x})}{\Delta x_i} & k = 1, \dots, p \end{aligned} \quad (2-46)$$

again with

$$\Delta \mathbf{x}_i = [0, 0, \dots, \Delta x_i, \dots, 0]^T$$

A new CFD simulation is required to approximate each of the gradients. A number of  $n + 1$  CFD simulations have therefore to be performed at each optimisation iteration. The restart feature of the CFD package can be used to reduce the computation time required to obtain the CFD solution. In some cases, the amount of iterations to obtain a converged CFD solution can be reduced by a factor of ten when using the restart feature of the CFD package.



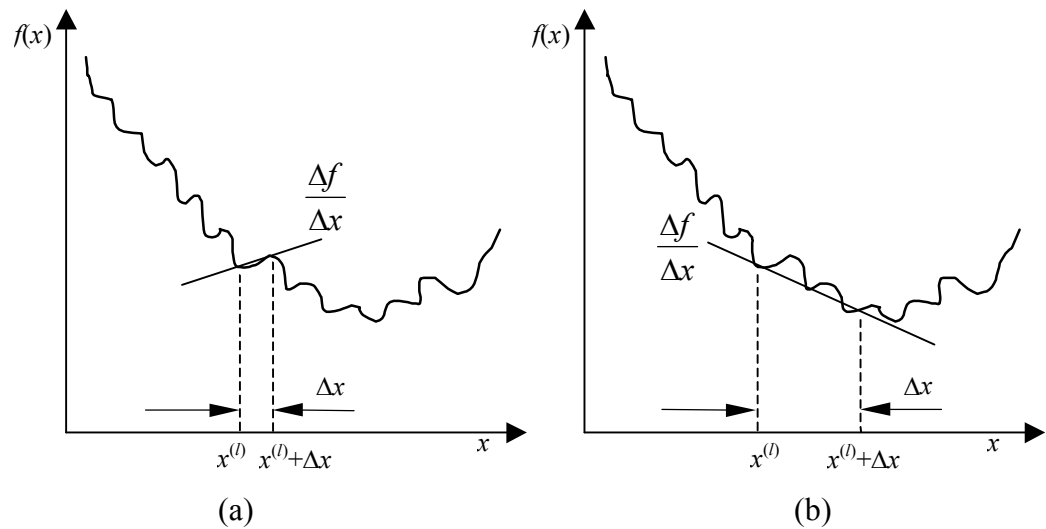
### **2-3.5 Effect of Noise Associated with CFD Solutions on the Gradient Approximation**

#### **2-3.5.1 Source of Noise in CFD Solutions**

In a steady-state CFD solution, the simulation is terminated when the residuals fall below a specified value. The numerical solution is therefore not an exact solution. Furthermore, there may be some round-off error due to the precision of the computer. If too small a  $\Delta x$  is chosen, the function value of the base case and that of the perturbation falls within the accuracy of the numerical analysis and the forward first-order differencing becomes void.

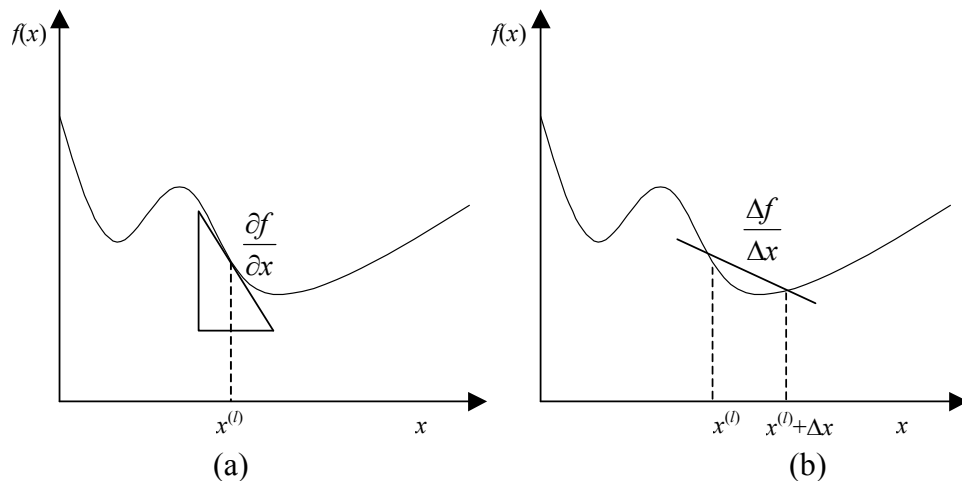
#### **2-3.5.2 Influence of Noise on the Finite Differencing Scheme**

Some difficulties may be encountered when approximating the derivatives using a finite differencing scheme on a noisy function. Figure 2-4 shows the effect on the first-order derivative when approximating the derivative using a forward-differencing scheme on a noisy function in one dimension. Figure 2-4(a) shows the approximated gradient for a small  $\Delta x$ . Due to the noise on the function, the gradient with a small  $\Delta x$  gives a totally different value than the one with a large  $\Delta x$  as shown in the right-hand graph of Figure 2-4(b). The gradient in the first graph is more accurate than the gradient in the second graph at point  $x^{(l)}$ , but when the subproblem is constructed using the gradient of the first graph, the optimisation will clearly end up with a wrong answer. The wavelength of the noise is closely linked to the correct choice of  $\Delta x$ . It is therefore desirable to choose a larger  $\Delta x$  so that the noise does not influence the global gradient of the function. Although the smaller  $\Delta x$  gives a more accurate gradient of the function, a larger  $\Delta x$  will give a more representative gradient when looking globally at the function.



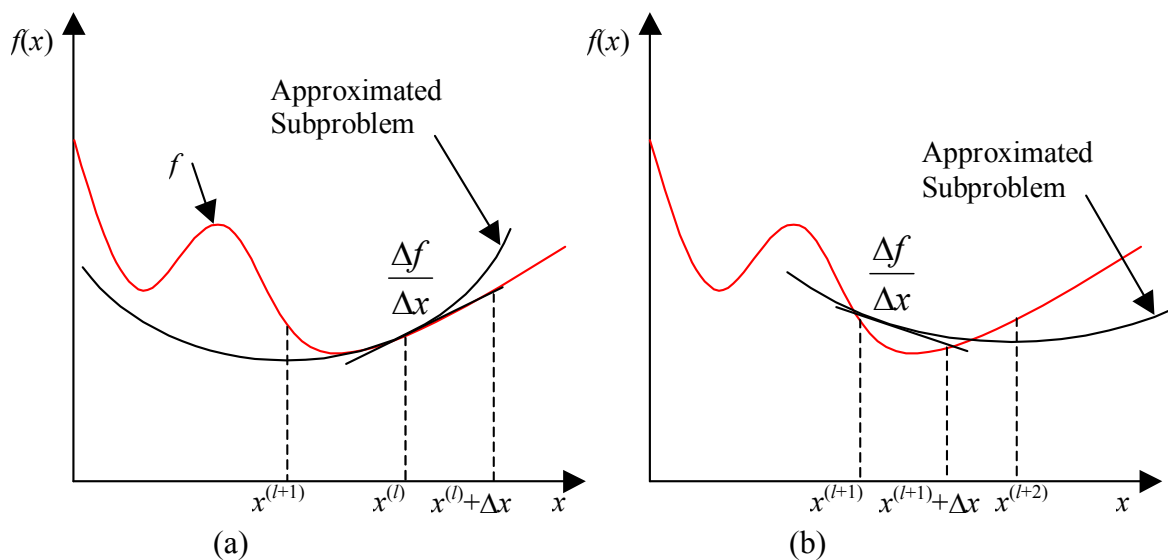
**Figure 2-4: Influence of a too small step size on the finite difference approximation of the gradients of a “noisy” function in 1-D**

Care must however be taken not to choose a too large  $\Delta x$ . This concept is illustrated in Figure 2-5 in 1-D. Choosing a too large  $\Delta x$  will result in an inaccurate gradient approximation as shown in Figure 2-5(b) compared to the true gradient as shown in Figure 2-5(a). The noise on the objective function, although present, is not shown in this figure.



**Figure 2-5: Influence of too large step size on the finite difference approximation of the gradients of a function in 1-D**

A large  $\Delta x$  may also cause the optimisation problem not to converge and cause the design variables to rock back-and-forth near the optimum. This is illustrated graphically in one dimension in Figure 2-6. The two graphs ((a) and (b)) shown in this figure depict two consecutive design points. Figure 2-6(a), the optimiser starts at point  $x^{(l)}$  and calculates a positive gradient of the function objective function,  $f$ , due to the forward-differencing scheme. The optimiser will then predict a smaller value for  $x$ . The new value  $x^{(l+1)}$  as prescribed by the optimiser will however result in a larger function value. As shown in Figure 2-6(b), the optimiser now calculates a negative gradient at point  $x^{(l+1)}$ , that will predict a larger value for  $x$ . The optimiser now moves to point  $x^{(l+2)}$ , which is just to the right of the original point  $x^{(l)}$ . This ‘rocking’ or cyclic motion may continue indefinitely until the optimiser is stopped.



**Figure 2-6: Rocking motion of one design variable near the optimum caused by the forward differencing scheme**

The right choice of  $\Delta x$  for each of the design variables will come from a sensitivity analysis. The sensitivity analysis is computationally very expensive and usually a good engineering estimate of an appropriate perturbation size will suffice. A general rule of thumb is to use a perturbation size of about 1/10 of the range of the design variable

There may be a variety of sources that cause the noise in the CFD solutions. This noise may be due to grid changes, convergence, numerical accuracy of the computer etc. This noise and the source of the noise still need some further investigation and falls outside the scope of this study. The better resolved the CFD analysis are, i.e., the finer the mesh, the higher the convergence of the residuals, and the more accurate the models used, the less contribution of noise is expected to be.

## **2-4 CONCLUSION**

The first part of this chapter described the current available literature on tundish and tundish furniture design. A large amount of research has been done on improving the design of tundish and tundish furniture. These improvements are achieved by using two different types of modelling techniques. The modelling is either through physical modelling or through numerical modelling. In the physical modelling, either plant trials or water models are used. Numerical modelling makes use of Computational Fluid Dynamics (CFD). The chapter looked in detail at the techniques, methods and procedures used in CFD to model different aspects of the tundish like turbulence, heat transfer and inclusion removal. All the cases in the literature in which new tundish or tundish furniture have been designed used a trial-and-error method to improve the design using either of the modelling techniques mentioned above.

The second part of the chapter focussed on mathematical optimisation. Mathematical optimisation was formally defined and then three optimisation algorithms were discussed. The effect of numerical noise inherent to a CFD analysis and its effect on gradient-based optimisation algorithms were also shown.

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## CHAPTER 3: TUNDISH DESIGN OPTIMISATION METHODOLOGY

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### 3-1 INTRODUCTION

This chapter describes the methodology developed to optimise tundish and tundish furniture designs. This chapter's aim is also to serve as a guide for the setup of an optimisation problem involving tundishes.

In order to optimise, one must first be confident that the modelling techniques used accurately predict the physical process being modelled. The first section of this chapter describes the validation of the modelling techniques that are going to be used to predict the physical process.

The next step is to formulate the optimisation problem. This is the most important step in the optimisation process. For the complex flow phenomena that exist inside a tundish, a wide range of candidate objective functions and constraints are available for possible use. It is up to the design engineer to decide which criteria and constraints are important and/or essential for his/her specific application.

The last section of the chapter describes the automisation of the optimisation procedure. This forms an essential part of the optimisation process. It is necessary for the optimisation procedure to be executed without any human intervention. This involves the automated setup of the problem being solved, solving the problem and then post-processing the results needed by the optimiser.

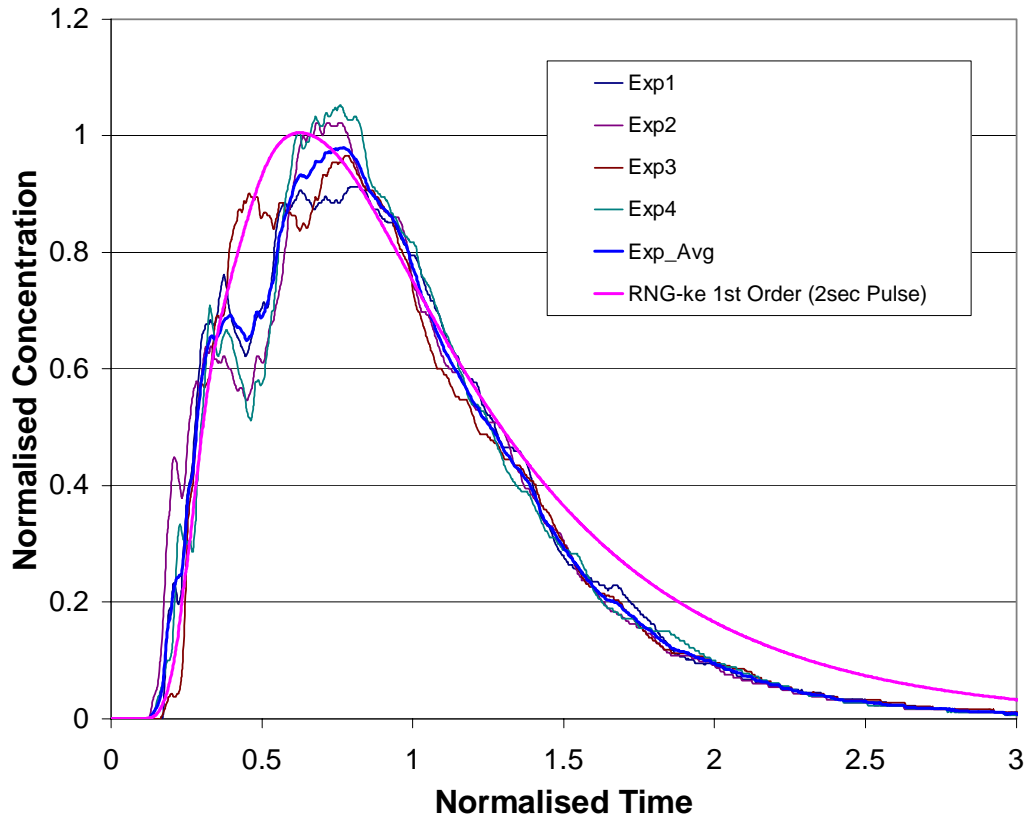
## **3-2 VALIDATION OF CFD MODEL**

A crucial prerequisite before an optimisation run can be started is to have confidence in the accuracy of the modelling tool used in the evaluation of the objective and constraint functions. The optimisation results can only be as good as the accuracy of the modelling. For this reason, two validation cases were undertaken to validate the CFD models. These two validation cases are described below.

### **3-2.1 Validation Case 1**

The first validation study undertaken was the validation against a full-scale single-strand water model of the Columbus Stainless Steel Caster. The details of this validation are given in Appendix A [65,66]. In this study a tracer was injected into the tundish at the shroud (refer Figure 1-1) and the concentration was measured at the outlet with a spectrophotometer [67]. The resulting Residence Time Distribution (RTD) curve was then compared with the numerical model as shown in Figure 3-1 (a repeat of Figure A-3, for ease of reference).

From the RTD curve, the relevant RTD data were extracted to compare with the experimental and CFD data. These data are given in Table 3-1 (repeated from Table A-1). Generally, good agreement is found between the experimental and CFD data with the minimum residence time (MRT) being the only value that is not predicted to within 15%. This MRT is however very sensitive to the duration of the injection and the sensitivity of the spectrophotometer (refer Appendix A).



**Figure 3-1: Comparison of RTD curves of the water model and CFD model**

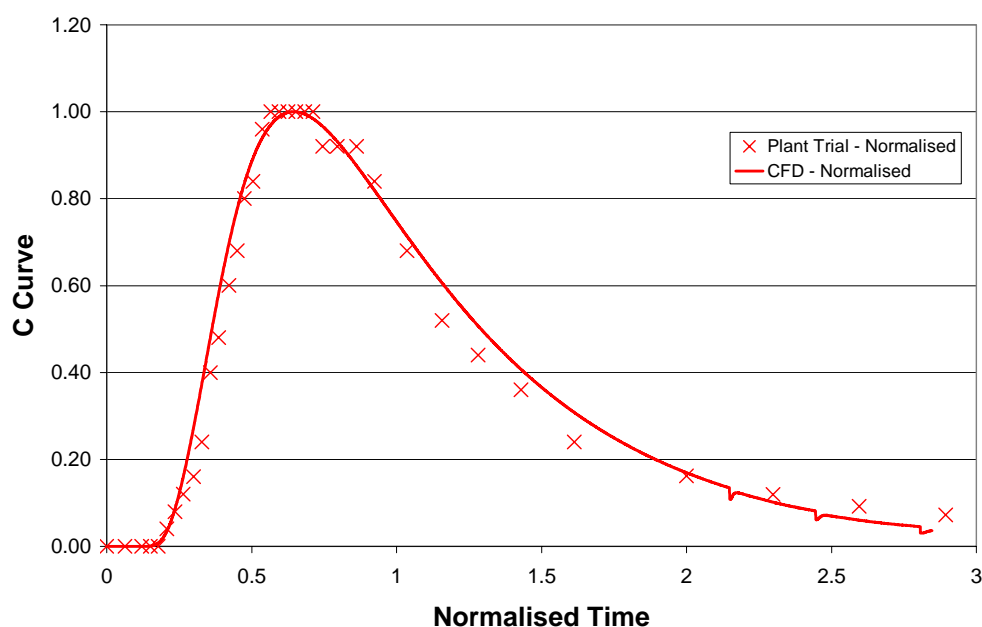
**Table 3-1: Comparison of RTD data of the water model and CFD model**

	Water model	CFD	% Difference
MRT	0.128	0.154	20.3%
Dispersed Plug Flow ( $V_{dpv}$ )	0.450	0.391	13.1%
Mixed Flow ( $V_{mv}$ )	0.406	0.452	11.3%
Dead Volume ( $V_{dv}$ )	0.144	0.156	8.3%

### **3-2.2 Validation Case 2**

The second validation was against a copper trace in a plant trial. The details of this validation study are given Appendix B [68]. This trial involved the introduction of copper adjacent to the shroud of the tundish and then

periodically taking samples from the mould. The copper concentration in the samples is then measured using a photospectrometer. This gives a RTD curve for the tundish that can be compared to that of the numerical model as given in Figure 3-2 (repeated from Figure B-2) and Table 3-2 (repeated from Table B-1). It can be seen from this figure and table that the plant trial and CFD are in good agreement. The dead flow volume is the only value that differs significantly with the plant trial results. The comparison is however acceptable, taking into account all the uncertainties associated with the plant trial.



**Figure 3-2: Comparison of RTD curves of the plant trial and CFD model**

**Table 3-2: Comparison of RTD data of the plant trial and CFD model**

	Plant Trial	CFD	% Error
Plug flow volume [%]	20.7	18.2	11.9
Mixed flow volume [%]	74.5	75.7	1.6
Dead flow volume [%]	4.8	6.1	27.1



### **3-3 FORMULATION OF OPTIMISATION PROBLEM**

The correct formulation of the optimisation problem is the most important step in any optimisation study. This section shows the different design variables, objective functions and constraints that can be chosen by the design engineer when optimising a tundish and tundish furniture.

#### **3-3.1 Candidate design variables**

The design variables are usually the easiest for the design engineer to choose. The variables are usually the design parameters that the engineer can and want to change to improve the design. Design variables for a tundish can be divided into two main categories, i.e., process variables and geometric variables.

The process variables include parameters like flow rate, inlet temperature, etc. Process variables are usually not as easy to change as these are dictated by the operation of the plant. For example, the molten steel inlet temperature is usually a function of the holding time of the ladle and the amount of time the ladle spent at the secondary metallurgy station.

Geometric variables include parameters like the position and height of a dam, or the shape and size of an impact pad or even the total size and shape of a tundish. The geometric variables, especially those linked to refractory components, are parameters that are easier to change and control than the process parameters.

#### **3-3.2 Candidate Objective Functions and Constraints from CFD analysis**

A number of candidate objective functions are available when optimising the tundish and tundish furniture design. A list of possible functions and their effect on the performance of the tundish are given below.

### **3-3.2.1 RTD Curve**

As shown in section 2-2.2, various quantities can be extracted from a RTD curve to determine the performance of the tundish. The different quantities and their possible use in an optimisation formulation are given below.

#### *Minimum Residence Time (MRT)*

The MRT or minimum break-through time, one typically wants as long as possible. A long MRT indicates a large plug flow volume and therefore smaller mixed volume and dead volume compared to a tundish with a short MRT. This in turn will result in a short mixed-grade length in the slab when casting different grades due to the lower mixed and dead volumes. Therefore, for the design of a tundish that will undergo many grade changes, the design engineer would want to maximise MRT.

#### *Well-mixed volume*

The well-mixed volume gives an indication to how much mixing takes place within the tundish. For inclusion particle removal, it is desirable to have a large amount of mixing as this give the particle the opportunity to reach the slag surface. Conversely, for a short mixed-grade length in the slab it is desirable to have a small amount of mixing. Therefore, for the design of a tundish where the quality is of high importance, the design engineer will want to maximise the well-mixed volume.

#### *Dead volume*

The dead volume gives an indication of stagnant or recirculating regions. These regions want to be kept as small as possible as this will negatively influence the length of the mixed-grade slab. The optimisation formulation would therefore be to minimise the dead volume.

Usually a trade-off has to be made between the MRT, well-mixed volume and dead volume. A tundish with very little mixing (i.e., a high MRT, low dead volume) gives a short mixed-grade length but low inclusion removal capabilities. On the contrary, a tundish with high mixing (i.e., a high well-mixed volume) will give good inclusion removal capabilities but a long mixed-grade length. It is the design engineer's responsibility to decide which is the most important in his/her specific application and choose the appropriate RTD related quantity.

### **3-3.2.2 Inclusion removal**

For higher quality steel and less defects, the design engineer will opt to maximise the inclusion removal on the slag layer. The inclusion removal modelling can be performed using the methods discussed in section 2-2.4.4. In some cases only the larger sized inclusions' (typically larger than 50micron) removal can be chosen to be maximised as the smaller inclusion (typically smaller than 50micron) will not adversely affect the quality of the steel. The inclusions are removed by sticking to the refractories and absorption into and reaction with the slag layer.

### **3-3.2.3 Mixed-grade length**

The mixed-grade length can be modelled explicitly by doing a transient multi-phase CFD analysis to capture the free surface between the air, slag layer and steel. This must be done to capture the effect of wave formation on the free surface and mixing of the inlet stream with the remaining steel as the tundish is filled with a different steel grade from a new ladle. As the multi-phase analysis is a computationally expensive, an indication of the mixed grade length can however be obtained from a RTD curve (discussed in section 3-3.2.1 above) obtained for a full level or using quasi-steady solutions at various fixed fill levels. This will not be as accurate as doing a multi-phase analysis.

The mixed-grade length will obviously be minimised to reduce the amount of steel that will be downgraded.

#### **3-3.2.4 Temperature**

The minimum temperature in the tundish is required to stay above a specified lower value. This is required so that the steel does not solidify inside the tundish. Furthermore, the tundish outlet temperature is required to be within a specified temperature range to carry a certain amount of super heat into the mould. These temperatures will typically be constraint functions that will be specified in the optimisation formulation.

#### **3-3.2.5 Slag layer**

It is required that the slag layer is stagnant and that turbulence levels on the slag layer are low. High velocities and turbulence levels on the slag layer might cause slag entrainment into the steel and adversely affect the quality of the steel. Another two possible objective functions would therefore be to minimise the turbulence levels on the slag layer or to minimise the velocities on the slag layer.

#### **3-3.2.6 Cascading**

Cascading happens during the first cast when the steel enters the tundish for the first time. During this time, there is no slag cover present and at these high temperatures, significant oxidation occurs. This oxidation results in a poor quality first slab. A possible optimisation formulation would therefore be to minimise the area of steel exposed to the atmosphere. This requires a transient multi-phase flow analysis of the filling that is computationally very expensive and probably not a viable formulation due to the excessive computational effort that will be required.

### **3-3.3 Other Constraints**

Other constraint functions also exist that are not related to the CFD simulation. These constraints are typical geometric constraints as well as manufacturing constraints. A typical manufacturing constraint would be the minimum thickness that a piece of tundish furniture could be. A geometrical constraint can also be derived from the required strength of the specific furniture piece, e.g., what is the minimum thickness that will withstand the ferrostatic head.

Another type of constraint that can be important is the yield that can be achieved by the tundish (i.e., minimising the liquid steel that remains in the tundish when drained). This can be based on a purely geometrical consideration or it can be based on the fact that a vortex forms at the end of a cast when the tundish level drops. The vortex then entrains slag that goes directly into the mould.

## **3-4 AUTOMATION OF OPTIMISATION PROBLEM**

The automation of the optimisation problem forms an important part of the whole optimisation procedure. The automation is done so that no human intervention is required once the optimisation process has started. The optimisation process is shown in the flow diagram given in Figure 3-3. For a given starting design ( $\mathbf{x}$ ), the mathematical optimiser generates a set of  $k$  designs that need to be evaluated. The number  $k$  and the exact values of the design vector to be evaluated ( $\mathbf{x}_i$ ) are a function of the specific optimiser to be used. A journal file for the specific design is then generated and is passed to GAMBIT (*gambit.jou*) to generate the geometry and the mesh to be used in FLUENT. The mesh is exported to FLUENT where another journal file (*fluent.jou*) controls the setting up, running and writing of the necessary files for the post-processing of the design. As an example in this flow diagram, a file called *conc.out* is written to the hard disk containing the outlet concentration. The output file(s) are then processed to yield the objective and constraint functions of the specific design. The mathematical optimiser gathers all these data and predicts a new optimum design. The process is repeated until the optimisation converges to specified criteria.

To reduce the time required by the optimiser to reach convergence, either the FLUENT simulation can be run in parallel on a multi-CPU machine or a cluster of machines on a Local Area Network; or each design to be evaluated ( $x_i$ ) can be run on a different computer. Both these methods will reduce the wall-clock time for one optimisation iteration.

The flow diagram in Figure 3-3 is applicable to both optimisers used in this thesis. The Dynamic-Q program of Snyman was adapted to be integrated into FLUENT and GAMBIT. The modified Fortran program is given in Appendix C.

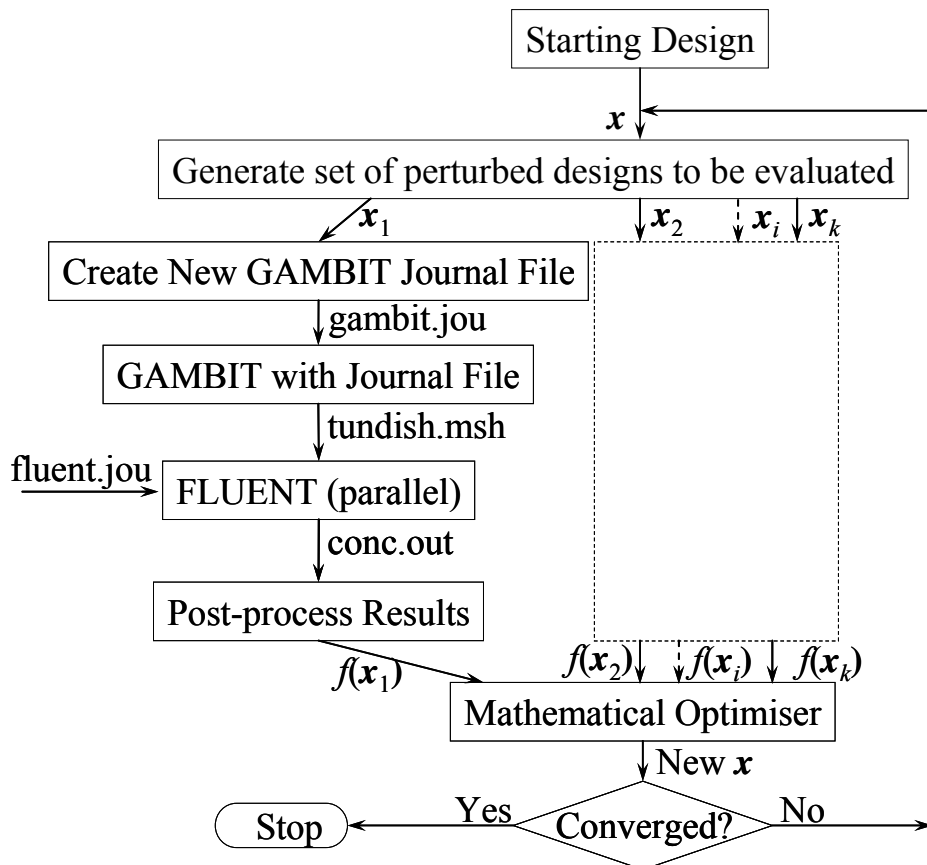


Figure 3-3: Flow diagram of FLUENT coupled to optimiser

### 3-5 CONCLUSION

This chapter described the methodologies investigated and developed to optimise tundish and tundish furniture. The first part of the methodology is to validate the

numerical model that will be used in the optimisation study. Secondly and the most important, is formulating the optimisation problem. This involves choosing the design variables and the appropriate object function and constraints. Typical design variables, objective function and constraint functions for tundish design were given and discussed. Lastly, the automation of the numerical set-up, solving and extraction of data were described. The following chapter will describe the application of this methodology to different case studies.

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## CHAPTER 4: APPLICATION OF TUNDISH DESIGN METHODOLOGY TO CASE STUDIES

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### 4-1 INTRODUCTION

The design optimisation methodology developed in Chapter 3 has been tested on a number of different case studies. These case studies are given in detail in this chapter. The chapter starts with the optimisation of a simple 1-dam-1-weir configuration. The optimisation of a baffle follows next, with the optimisation of an impact pad and an impact pad with a dam forming the last two test cases.

### 4-2 CASE STUDY 1: OPTIMISATION OF 1-DAM-1-WEIR CONFIGURATION

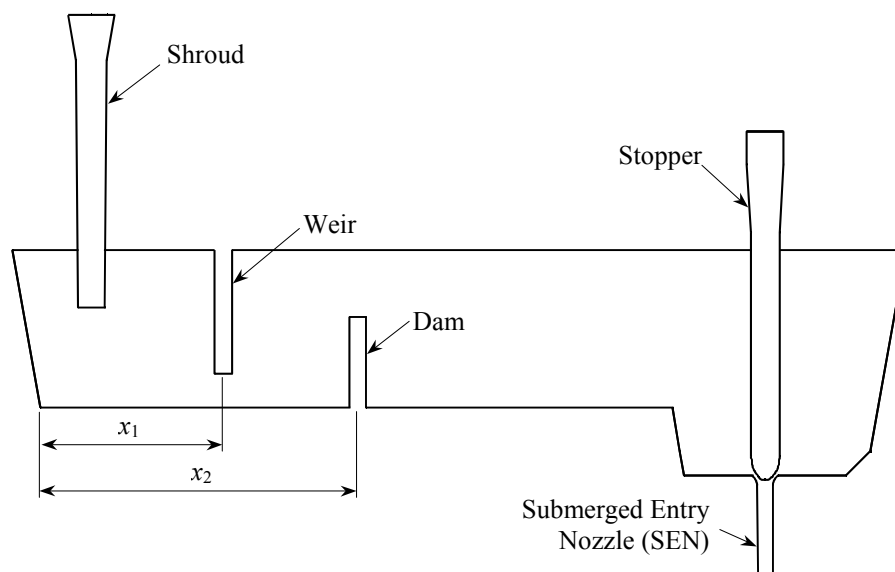
The first case study involves the single-strand stainless steel continuous caster in operation at the Middelburg plant of Columbus Stainless. The work of this case study has been published in the Journal of Iron and Steel Institute of Japan International [69] and presented at the 20<sup>th</sup> International Congress of Theoretical and Applied Mechanics [70].

The tundish geometry considered is shown in Figure 4-1. The flow rate is controlled by the position of the stopper. When injecting a tracer element at the shroud (inlet), this tracer is detected at the SEN (outlet) after a certain amount of time. The concentration at the outlet increases to a maximum where after it decreases. The time history of the tracer concentration as measured at the outlet is called the Residence Time Distribution (RTD) in 2-2.2. The rate of decay is of interest since it correlates with the ratio of plug flow versus mixed flow in the tundish. The amount of tracer left in the tundish after  $2\bar{t}$  (twice the mean residence time) is defined in this study as the



dead volume, and is minimised in the first optimisation problem. The second optimisation problem considers the removal of inclusion particles.

As mentioned before, a water model validation study was also undertaken on this specific tundish geometry to ensure the accuracy of the numerical model. The water model tests were done on a full-scale tundish installed at the University of Pretoria by other members of the research group. The results of the water model test and those obtained with numerical model compared favourably. Details of the validation study are given in Appendix A. Water is used as the modelling fluid for the first case study.



**Figure 4-1: Side view of tundish showing dam, weir, stopper, SEN and shroud**

The complete mathematical formulation of the optimisation problems, in which the inequality constraints are written in the standard form  $g_j(\mathbf{x}) \leq 0$ , where  $\mathbf{x}$  denotes the vector of the design variables  $(x_1, x_2)^T$ , are as follows:

Case 1a: Minimise  $\left[ \begin{array}{l} f(\mathbf{x}) = \text{dead volume} \\ = 1 - (\text{concentration at } t = 2\bar{t}) \end{array} \right]$

subject to:  $\begin{cases} g_1 = -x_1 + x_1^{\min} \leq 0 \\ g_2 = x_1 - x_2 + \delta \leq 0 \\ g_3 = x_2 - x_2^{\max} \leq 0 \end{cases}$  (4-1)

where  $\delta$  is the minimum distance between the dam and the weir and  $x_1^{\min}$  and  $x_2^{\max}$  are the left most and right most positions of the weir and dam, respectively.

Case 1b: Minimise  $[f(\mathbf{x}) = \text{Percentage Escaped particles}]$

subject to:  $\begin{cases} g_1 = -x_1 + x_1^{\min} \leq 0 \\ g_2 = x_1 - x_2 + \delta \leq 0 \\ g_3 = x_2 - x_2^{\max} \leq 0 \end{cases}$  (4-2)

The results for the two cases of the 1-dam 1-weir configuration are presented next.

#### **4-2.1 Case 1a: Dead Volume Minimisation**

##### Parameters

The parameters used in this study are given in Table 4-1. The limits on the design variables and move limits are shown in Table 4-2.

**Table 4-1: Parameters used in the numerical model**

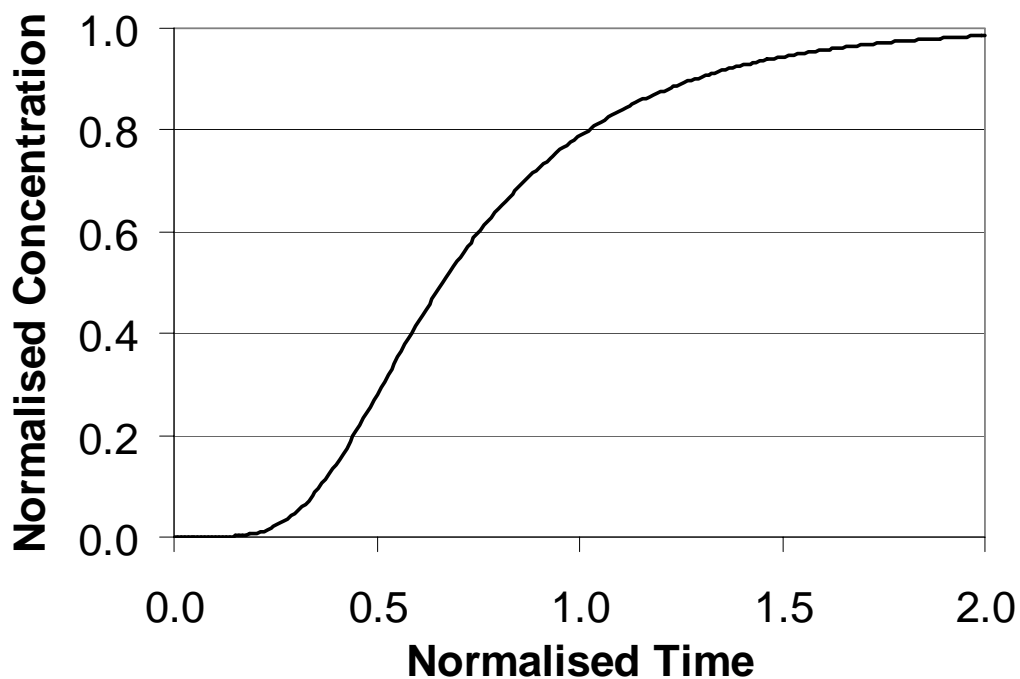
Parameter	Value
Mass Flow Rate [ $\text{kg}\cdot\text{s}^{-1}$ ]	4.75
Tundish Volume [ $\text{m}^3$ ]	2.05
Dead Volume Time [s]	$2\bar{t} = 1176$
Water density, $\rho_{\text{water}}$ [ $\text{kg}\cdot\text{m}^{-3}$ ]	998
Water Viscosity, $\mu_{\text{water}}$ [ $\text{kg}\cdot\text{m}^{-1}\cdot\text{s}^{-1}$ ]	0.00103
Minimum distance, $\delta$ [m]	0.2

**Table 4-2: Upper and lower limits and move limits on the design variables**

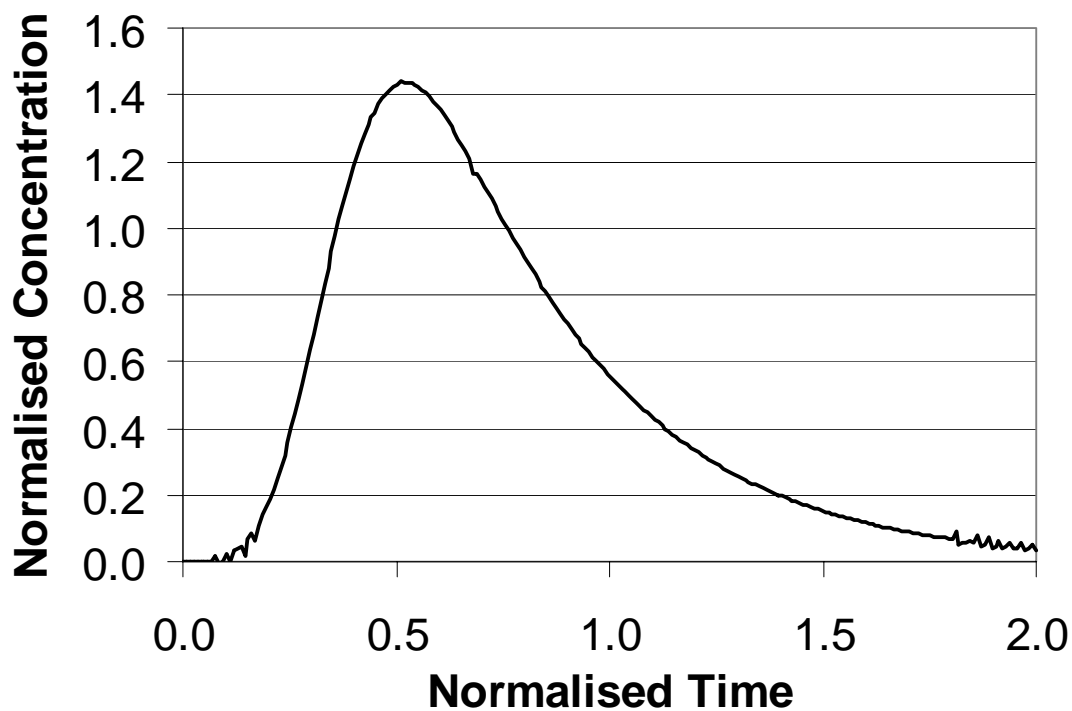
	Weir Position ( $x_1$ ) [m]	Dam Position ( $x_2$ ) [m]
Minimum	0.4629	-
Maximum	-	2.7266
Move Limit	0.5	0.5

Flow Results

The outlet concentration and the RTD curve for the initial design iteration ( $x_1 = 0.9$ ,  $x_2 = 1.5$ ) as obtained with a transient simulation are shown in Figure 4-2 and Figure 4-3 respectively. The curves end at  $\bar{t} = 2.0$ , i.e., 1176s = 19min35s. The dead volume is obtained from 1 minus the concentration at  $\bar{t} = 2.0$  in Figure 4-2, since the integral of the curve in Figure 4-3 is equal to 1.0.



**Figure 4-2: Concentration profile of starting configuration ( $x_1 = 0.9$ ,  $x_2 = 1.5$ )**



**Figure 4-3: RTD curve of starting configuration ( $x_1 = 0.9$ ,  $x_2 = 1.5$ )**

#### Optimisation Results

The results of Case1a are shown in Figure 4-4 and Figure 4-5. The history of the objective function is shown in Figure 4-4 while the history of the design variables is shown in Figure 4-5. A graphical representation of the optimum configuration is also shown in Figure 4-5. It can be seen that the first potential optimum is found in iteration 4, where after the optimiser diverges, but then recovers to find a slightly better minimum. At iteration 4, the constraint on  $x_1$  is only just not active, whereas from iteration 5 onwards, it remains active, with  $x_1$  at its lowest allowable value. Physically, this means that the design pushes the weir as close to the inlet as possible, while it searches for the optimum position of the dam, relatively close to the outlet. The main deduction that can be made from the optimisation results for this two-variable design problem, is that the dead volume is relatively insensitive to the position of the dam and weir. Although the dead volume has been reduced to nearly half its value in the initial design, the dead volume was very small to begin with (1.45%).

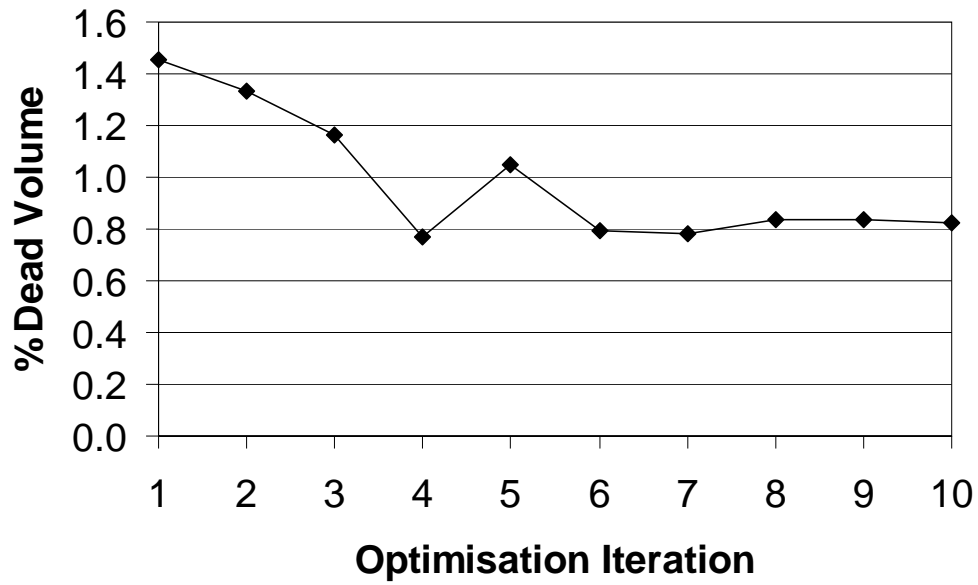


Figure 4-4: Optimisation history of objective function (Case 1a)

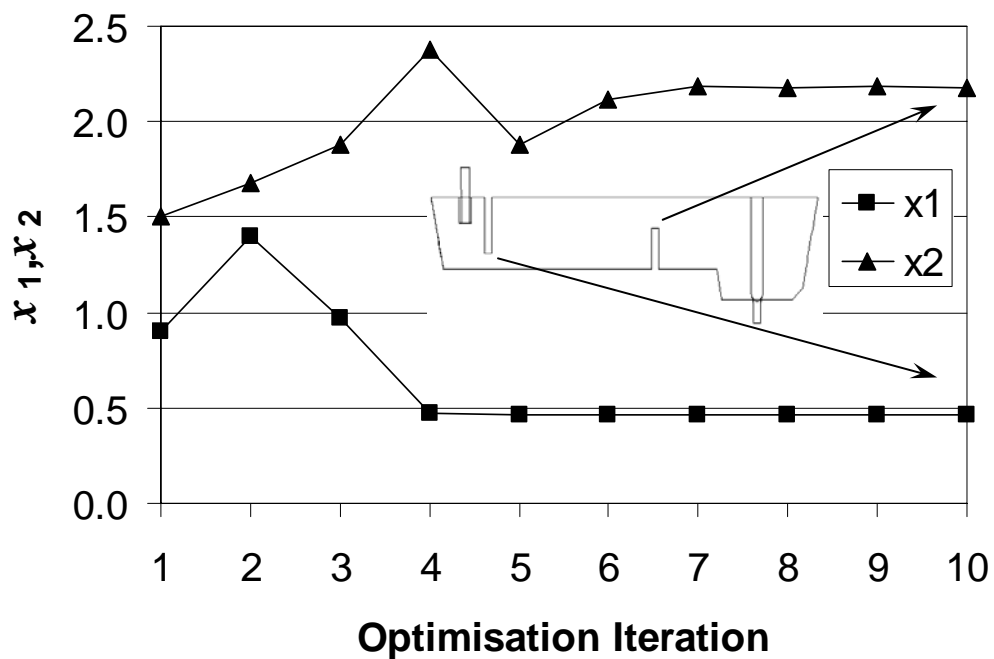


Figure 4-5: Optimisation history of design variables (Case 1a)

### **4-2.2 Case 1b: Inclusion Removal Optimisation**

#### Parameters

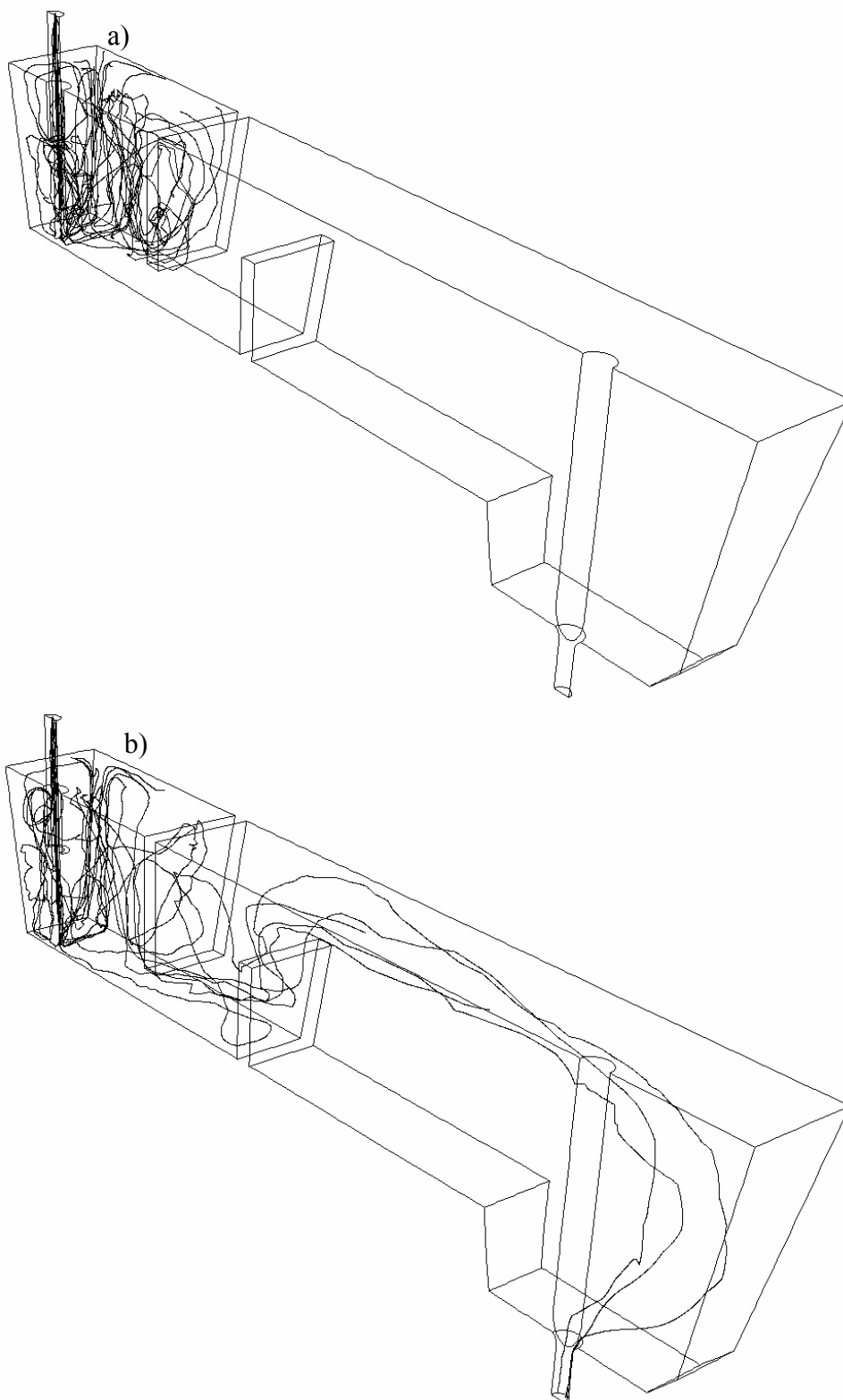
The same parameters and limits on the design variables are used as in Case 1a. The only additional parameters considered is the inclusion size distribution, inclusion particle mass flow and density. The inclusion size distribution is given in Table 4-3. These data were acquired from taking a sample of the steel at the shroud on the plant and then using an image analyser to determine the size distribution. This information was obtained from ISCOR Vanderbijlpark Works [71]. The mass flow is determined from the total percentage of inclusions in the sample and was calculated as  $0.469\text{g}\cdot\text{s}^{-1}$  for the whole tundish. The density of the inclusions was taken as  $456\text{kg}\cdot\text{m}^{-3}$  which is 2.2 times smaller than the density of the water (the modelling fluid used). This represents the same density ratio of the alumina inclusions relative to the molten steel in the plant. A total of 2700 inclusions with the same size distribution as in Table 4-3 are released in the CFD simulation.

**Table 4-3: Inclusions size distribution obtained from image analyser [71]**

Size [mm]	Number of particles
0.024	113
0.093	37.75
0.207	4.5
0.366	0.5
0.571	0.25

#### Inclusion Tracks

The inclusion tracks for the starting design are shown in Figure 4-6 for two of the inclusion sizes considered (i.e. 0.024mm and 0.207mm), released at one specific location for illustration purposes. It can be seen that the all the larger inclusion are trapped at the slag layer before the weir due to their larger buoyancy forces (Figure 4-6a). The smaller inclusions tend to follow the flow stream and exit at the SEN (Figure 4-6b).



**Figure 4-6: Particle tracks for a) 0.207mm b) 0.024mm size inclusions released at one specific location only (Starting configuration:  $x_1 = 0.9$ ,  $x_2 = 1.5$ )**

### Optimisation Results

The history of the inclusion optimisation is shown in Figure 4-7 and Figure 4-8. The history of the objective function is shown in Figure 4-8, while the history of the design variables is shown in Figure 4-8. It can be seen from Figure 4-8 that the optimiser tends to hit the constraint of minimum distance ( $\delta$ ) between the dam and the weir, and then moves the dam and weir together as a pair. A graphical representation of the optimum configuration is also shown in Figure 4-8. This small distance between the dam and the weir creates a jet with a high velocity directed towards the surface providing a mechanism for particle trapping. This may however cause some entrainment of the slag layer, which was not modelled in this case due to the absence of a free surface in the CFD model.

The reduction in the objective function is quite small as can be seen in Figure 4-7. This shows that the inclusion removal capability of this tundish with these given tundish furniture and constraints are not very good. Also, the improvements that can be made to the design to increase the inclusion removal capability are not great.

It can also be seen that this optimum differs completely from the optimum in Case 1a. The main reason for this is that the two objective functions represent two opposing design criteria.



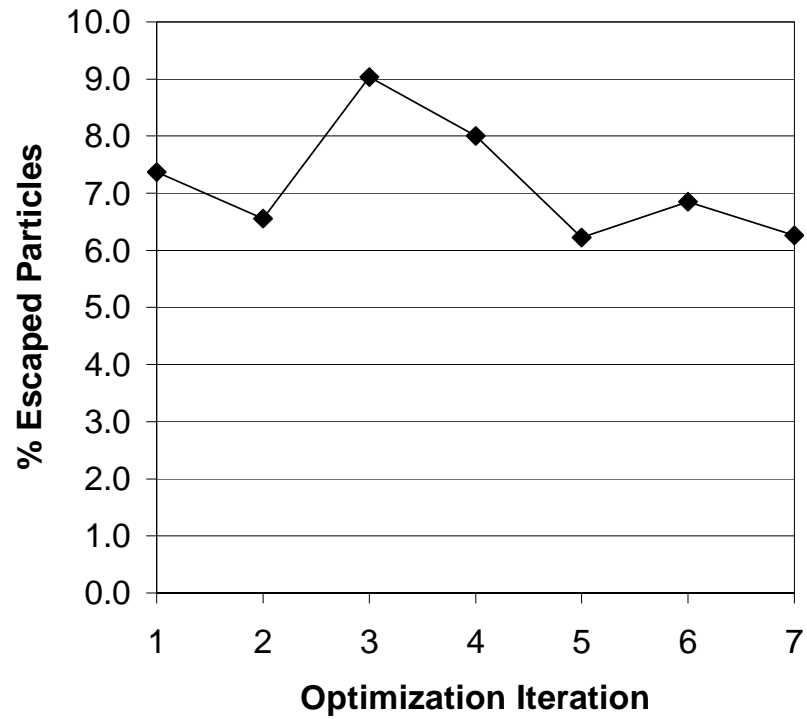


Figure 4-7: Optimisation history of the objective function (Case 1b)

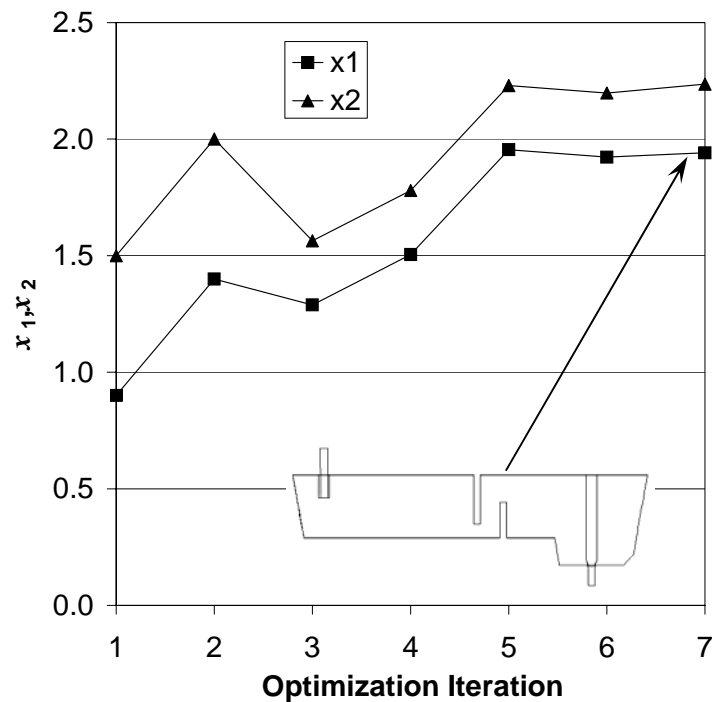


Figure 4-8: Optimisation history of the design variables (Case 1b)

### **4-2.3 Conclusion**

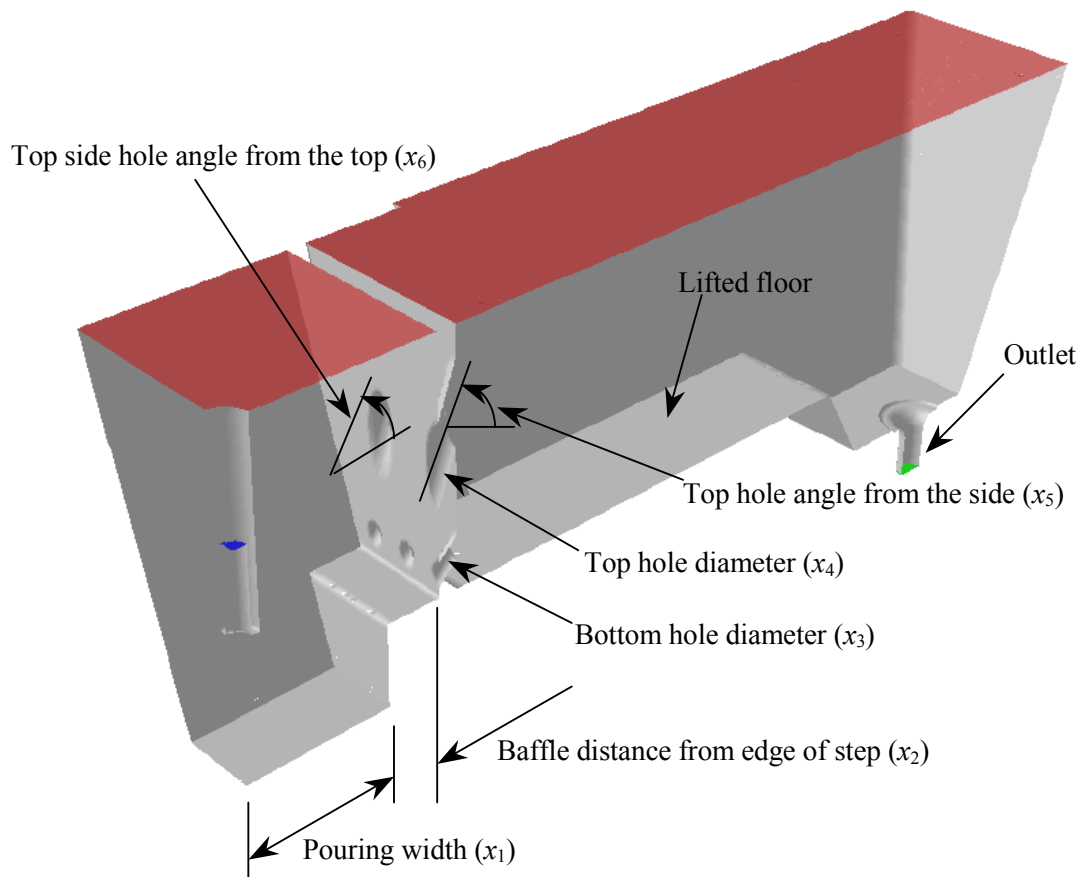
A simple dam and weir configuration was optimised for the single-strand continuous caster of Columbus Stainless Steel. Two different objective functions were defined for two different cases under investigation. It was shown that different optima exist for these different objective functions.

### **4-3 CASE STUDY 2: BAFFLE OPTIMISATION**

This study considers the two-strand continuous caster at ISCOR Vanderbijlpark Works, South Africa. ISCOR was in the process of enlarging the tundish capacity of their two-strand continuous caster from 40 tonnes to 60 tonnes. Part of the consideration of the increased capacity was to design the tundish and tundish furniture in order to improve steel quality. The main design criterion was to improve the cleanliness of the steel produced by this caster. This work has been presented at the 4<sup>th</sup> European Continuous Casting Conference [72] and published in the Ironmaking and Steelmaking journal [68].

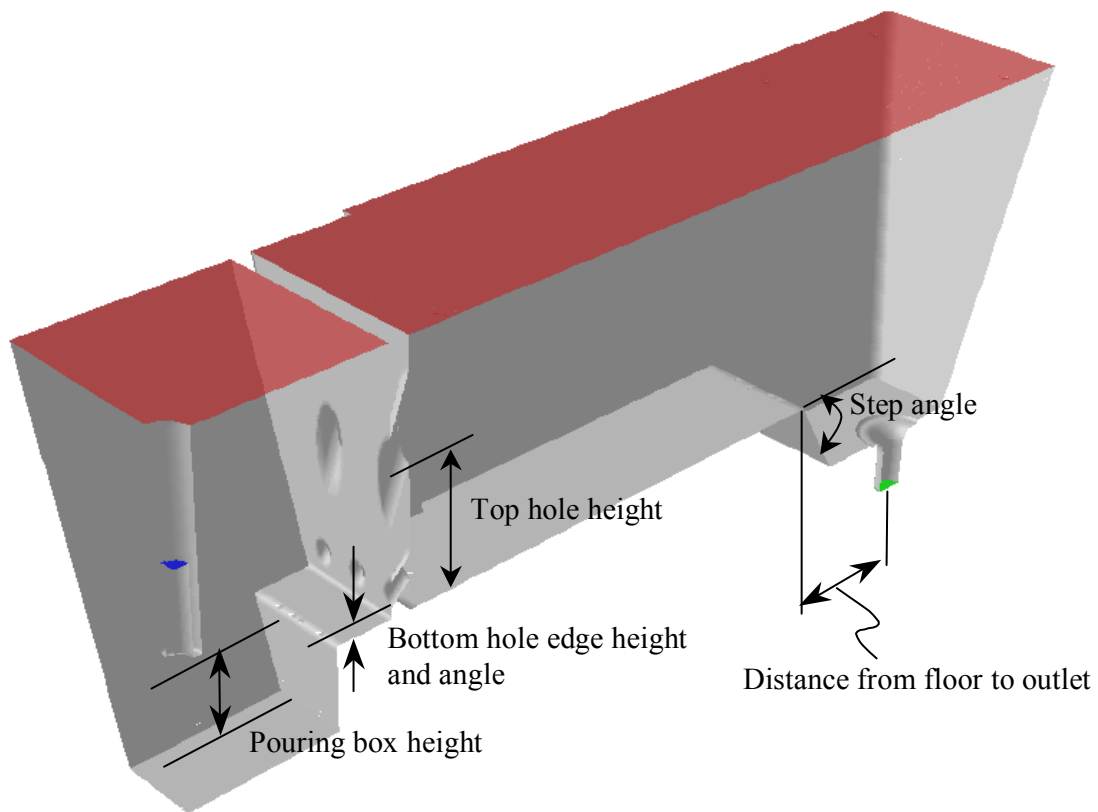
As the caster operates with long sequences, the Minimum Residence Time (MRT) of the tundish is maximised both at operating level and at a typical transition level of 700mm from the bottom of the tundish. A high MRT implies increased plug flow which has been linked to increased inclusion removal. In the numerical model, the MRT is obtained by injecting a passive scalar at the inlet and calculating the time it takes to appear at the outlet. The MRT is defined mathematically, as the non-dimensional time when the outlet concentration of the scalar reaches 0.1% of the constant inlet concentration. The time is non-dimensionalised using the theoretical mean residence time. The optimisation algorithms used in this case study (DYNAMIC-Q and LS-OPT) allow for one objective function. Therefore when two criteria are optimised, it is customary to consider a weighted combination as the objective function. Since the tundish operates predominantly at full level but quality during transition is also of concern, it was decided to combine the two respective MRTs in a 70:30 ratio.

Six geometrical variables of the tundish and tundish furniture are used as design variables. The six design variables are shown graphically in Figure 4-9.



**Figure 4-9: Graphical depiction of the design variables (1/4 symmetrical model) (Case 2)**

Apart from the design variables chosen, the values of other parameters that were held fixed during the optimisation are shown in Figure 4-10 and enumerated in Table 4-4.



**Figure 4-10: Fixed parameters for optimisation of tundish (1/4 symmetrical model) (Case 2)**

**Table 4-4: Fixed parameters of optimisation problem (Case 2)**

Parameter	Value
Bottom hole angle [°]	45
Pouring box height [mm]	300
Distance from floor to outlet [mm]	350
Step angle (at outlet) [°]	80
Bottom hole edge height (from lifted floor) [mm]	50
Top hole height (centre from lifted floor) [mm]	450

The complete mathematical formulation of the optimisation problem, in which the constraints are written in the standard form  $g(\mathbf{x}) \leq 0$ , where  $\mathbf{x}$  denotes the vector of the design variables  $(x_1, x_2, x_3, x_4, x_5, x_6)^T$ , is as follows:

$$\text{Maximise } [f(\mathbf{x}) = 0.7 \times MRT_{full}(\mathbf{x}) + 0.3 \times MRT_{700mm}(\mathbf{x})],$$

$$\text{subject to: } \begin{cases} g_j = -x_j + x_j^{\min} \leq 0; j = 1, 2, 3, \dots, n \\ g_{j+n} = x_j - x_j^{\max} \leq 0; j = 1, 2, 3, \dots, n \\ g_{2n+1} = \frac{x_4}{\cos x_5} + 70 \tan x_5 - 400 \leq 0 \end{cases} \quad (4-3)$$

where  $x_j^{\min}$  and  $x_j^{\max}$  are suitable minimum and maximum constraints or bounds for the  $j$ -component of the design vector,  $\mathbf{x}$ , and  $n = 6$ . The upper and lower bounds on the variables are given in Table 4-5. No upper bounds are placed on four of the variables. The last constraint in equation (4-3) is derived from the fact that the exit of the top hole should be 50mm below the full operating level of the tundish to prevent possible slag entrainment. For the 700mm level, this hole protrudes above the liquid steel level.

**Table 4-5: Minimum and maximum values of design variables (Case 2)**

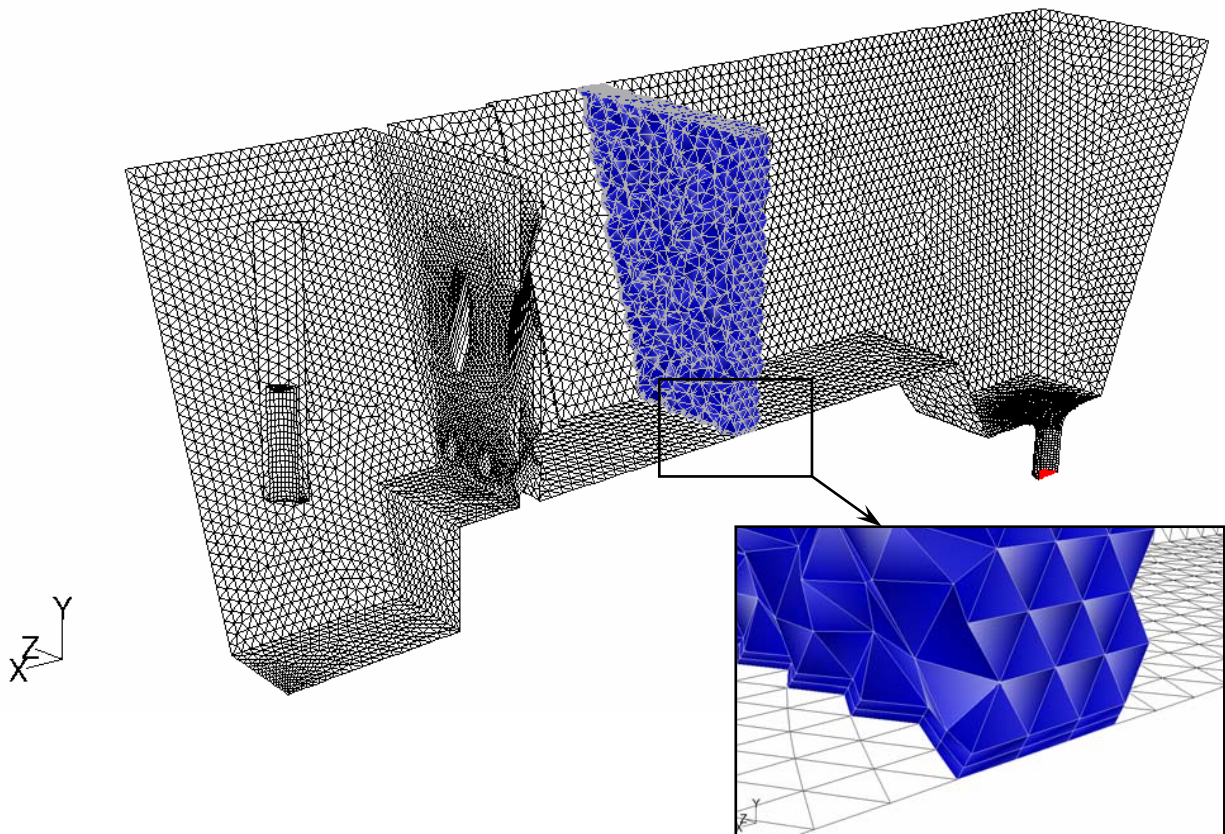
Variable	Minimum	Maximum	Starting Design
Pouring width ( $x_1$ ) [mm]	250	1075	300
Baffle distance ( $x_2$ ) [mm]	50	N/A	100
Bottom hole diameter ( $x_3$ ) [mm]	50	N/A	70
Top hole diameter ( $x_4$ ) [mm]	50	N/A	100
Top hole angle from side ( $x_5$ ) [°]	-70	N/A	70
Top hole angle from top ( $x_6$ ) [°]	-10	10	0

### **4-3.1 Flow Modelling**

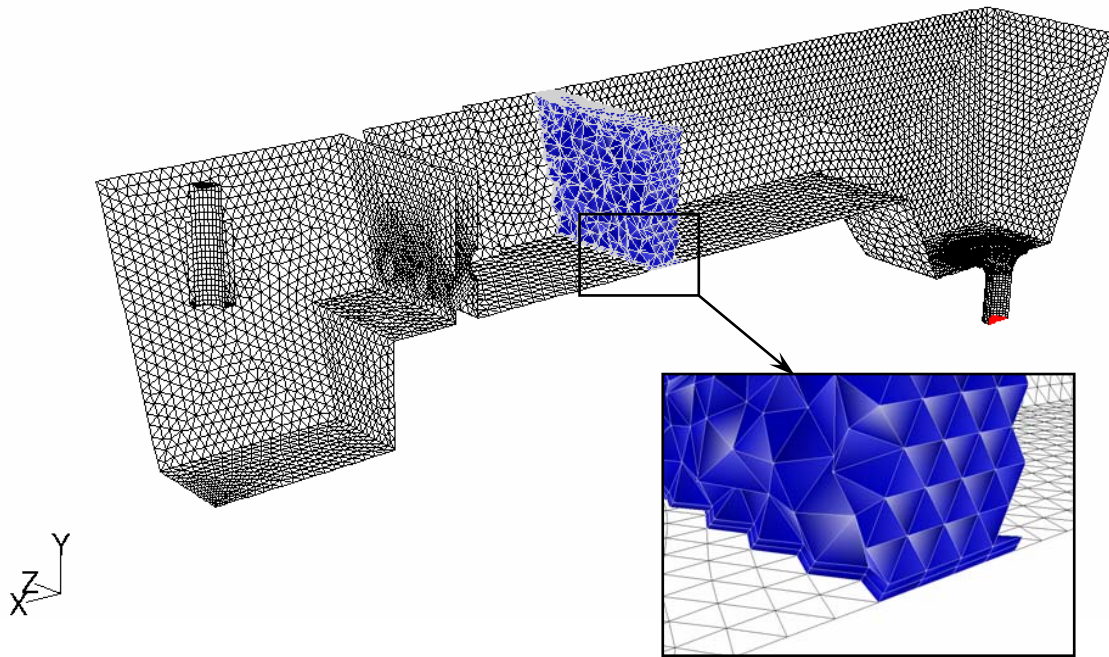
#### Grid

The grids used throughout the optimisation contained about 375 000 and 200 000 cells respectively for the full and half-full (700mm level) cases after refinement. Refinement was based on  $y^+$ -values to ensure the correct implementation of the wall-function approach used in the turbulence modelling [33]. A typical grid at operating level used in the optimisation is

shown in Figure 4-11 while a typical grid at transition level is give in Figure 4-12. A section of the internal cells is shown in these figures. A close-up of this section close to the wall is also given. It can be seen that tetrahedral cells combined with prisms cells at the wall boundaries were used. The prisms cells give a good quality mesh near the wall of the tundish for good representation of the moment and thermal boundary layer due to the no-slip condition on the wall.



**Figure 4-11: Typical grid at operating level (Case 2)**



**Figure 4-12: Typical grid at transition level (Case 2)**

Boundary Conditions and Fluid Properties

The boundary conditions used in the CFD model are shown in Figure 4-13. The effective heat transfer coefficients of the slag layer, side and bottom walls of the tundish are also indicated in Figure 4-13. These values were calculated using the thermal properties of the tundish walls given in Table 4-6 as well as experimental correlations [73] that determine the natural convective heat transfer and radiation on the outside walls of the tundish. The lifted floor of the tundish and the baffle are assumed to be adiabatic. The properties of the liquid steel used are given in Table 4-7.



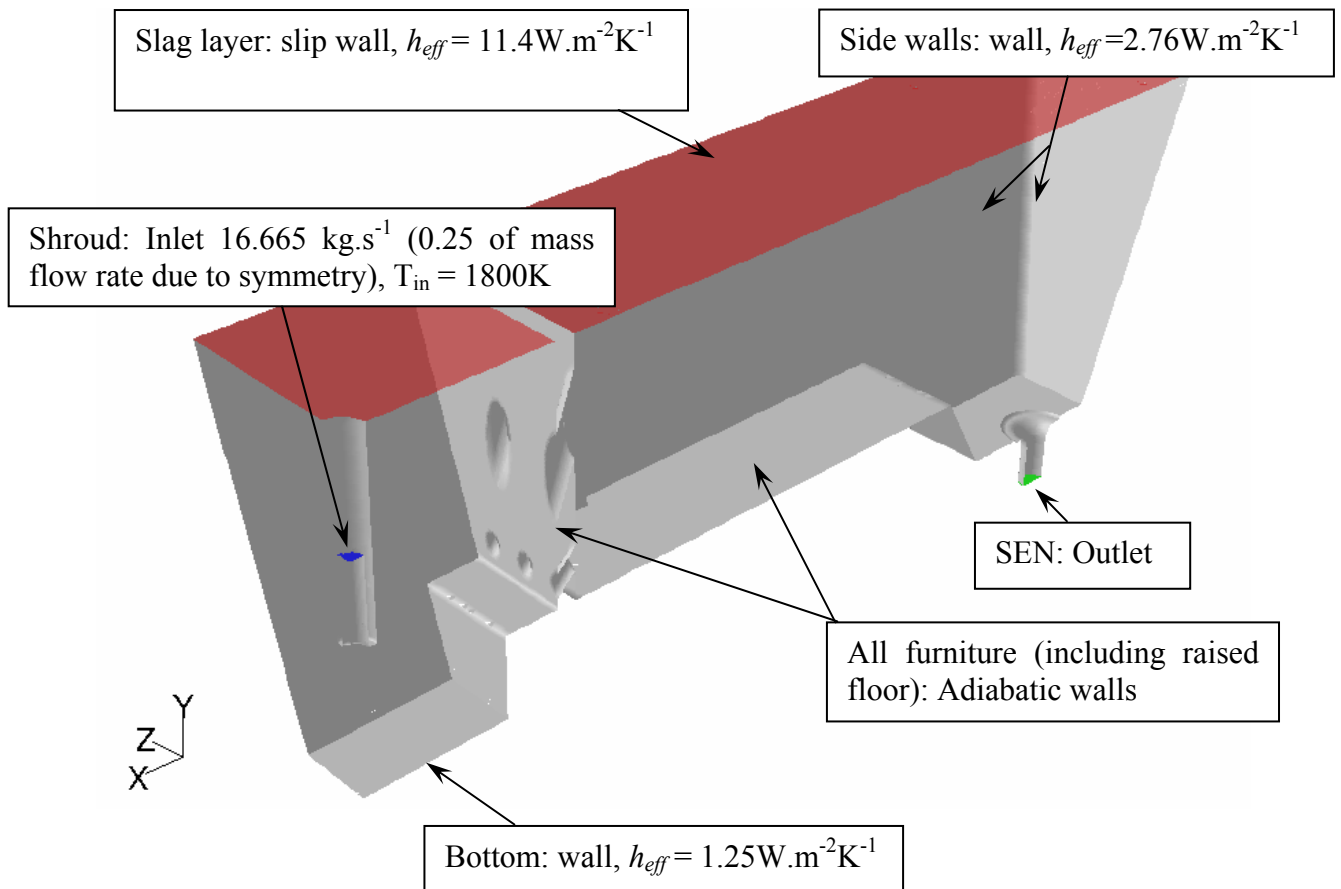


Figure 4-13: Boundary conditions used in tundish model (Case 2)

Table 4-6: Thermal properties of tundish (Case 2)

	Tundish construction	Insulation	Safety lining	Back lining	Work lining
Thickness [m]	0.03	0.025	0.025	0.114	0.04
Conductivity [ $\text{W.m}^{-1}.\text{K}^{-1}$ ]	72.93	0.15	1.48	1.57	1.65

**Table 4-7: Properties of liquid steel (Case 2)**

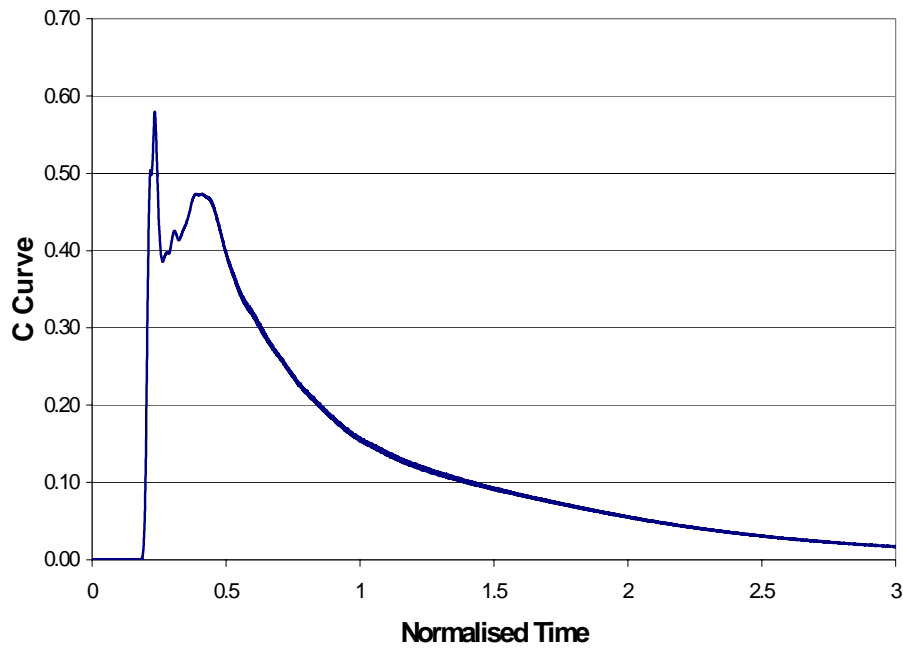
Property	Value
Thermal expansion coefficient [ $K^{-1}$ ]	$1.1970 \times 10^{-4}$
Reference density [ $kg.m^{-3}$ ]	7026.8
Reference temperature [K]	1800
Specific heat coefficient of steel [ $J.kg^{-1}.K^{-1}$ ]	822
Conductivity of liquid steel [ $W.m^{-1}.K^{-1}$ ]	52.535
Dynamic viscosity of steel [Pa.s]	$5.3 \times 10^{-3}$

### Solver

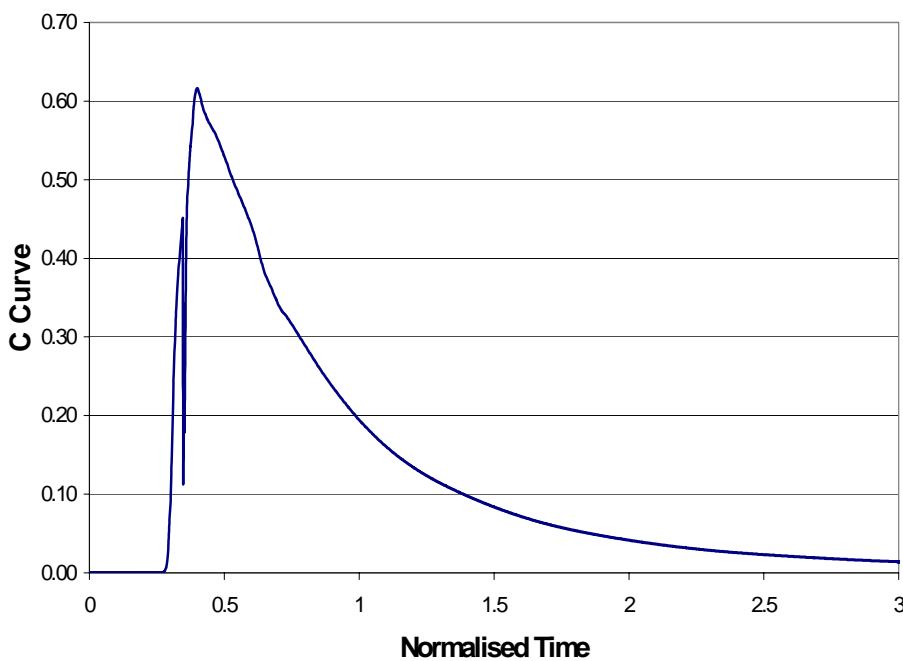
For the simulations presented in this study, the Reynolds-Averaged Navier-Stokes equations are solved using the segregated solver available in FLUENT. The standard  $k-\varepsilon$  turbulence model is used to provide turbulent closure. Second-order discretisation is used for all the flow equations while a three-order drop in the sum of the scaled residuals was considered to constitute a converged solution.

### **4-3.2 Flow Simulation Results**

Typical results obtained from the CFD simulations are given in this section. The starting design RTD curves for the operating level and transition level are given in Figure 4-14 and Figure 4-15 respectively. The spikes in the RTD curve are indicative of possible short-circuiting in the tundish. The RTD data for the starting design for the operating level and transition level are given in Table 4-8.



**Figure 4-14: RTD obtained from CFD simulation for starting design at operating level ( $x = (300,100,70,100,70,0)^T$  and MRT=0.189) (Case 2)**

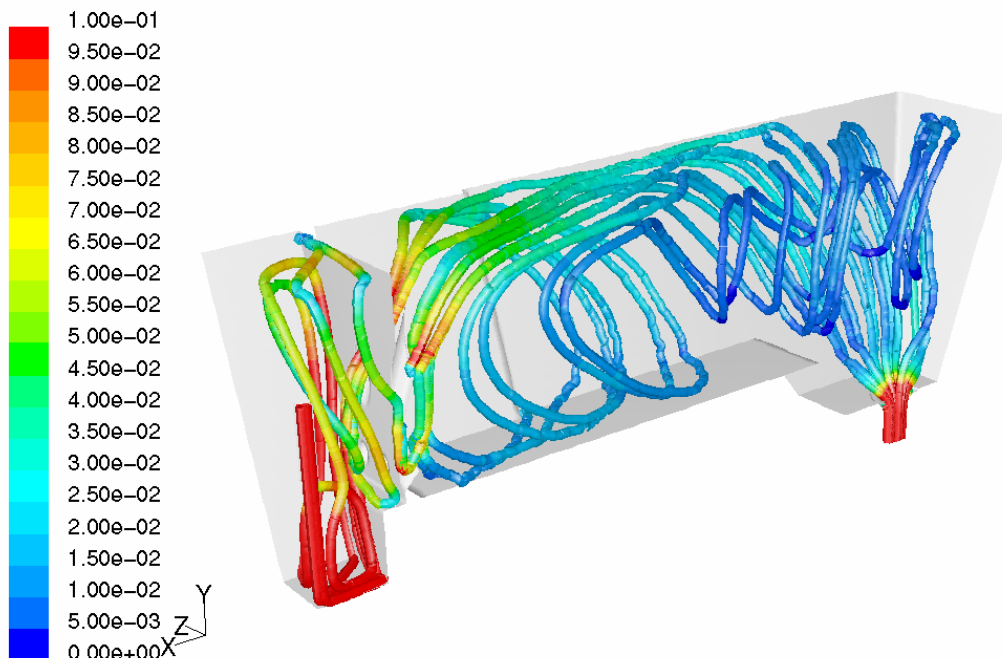


**Figure 4-15: RTD obtained from CFD simulation for starting design at transition level ( $x = (300,100,70,100,70,0)^T$  and MRT=0.283) (Case 2)**

**Table 4-8: RTD data for starting design ( $x = (300,100,70,100,70,0)^T$ )(Case 2)**

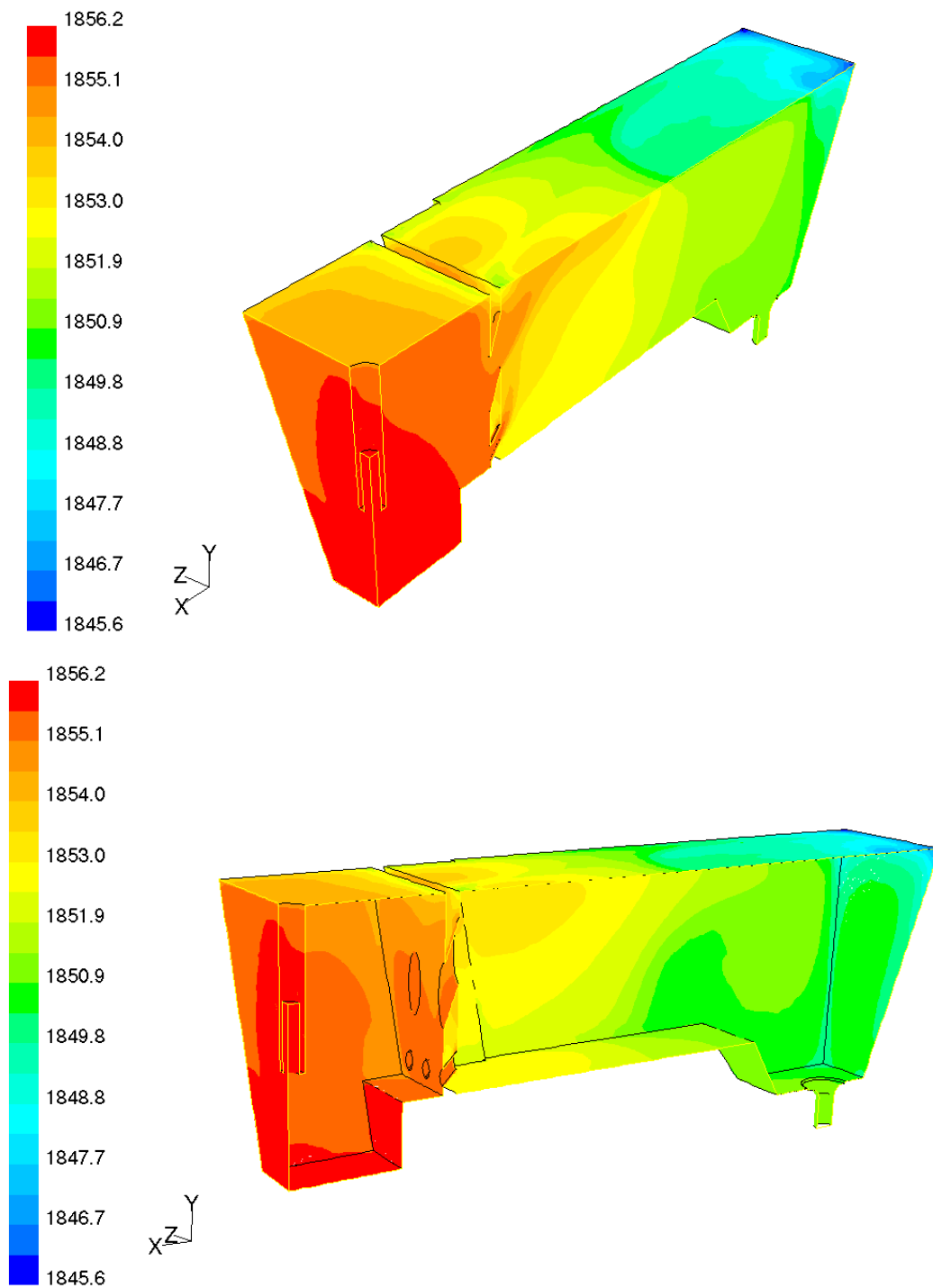
	Full	700mm Level
Dispersed Plug Flow [%]	21.2	34.2
Dead Volume [%]	23.2	19.9
Mixed Volume [%]	55.7	46.0
<b>MRT (non-dimensionalised)</b>	<b>0.189</b>	<b>0.283</b>
PRT (non-dimensionalised)	0.234	0.400
AMRT (non-dimensionalised)	0.768	0.801

Path lines for the starting design are given in Figure 4-16 for the full operating level. Figure 4-16 shows that the tundish flow exhibits a large recirculation zone behind the baffle. Temperature contours for the operating level are given in Figure 4-17. As expected, the steel is the hottest in the pouring box region, with the coolest regimes being in the cornets above the tundish outlet. The hot jet of steel that is caused by the baffle holes can also be clearly seen in Figure 4-17.



**Figure 4-16: Path lines coloured by velocity magnitude [ $\text{m}\cdot\text{s}^{-1}$ ] from CFD simulation at full operating level for starting design**

**( $x = (300,100,70,100,70,0)^T$  ) (Case 2)**



**Figure 4-17: Typical temperature contours [K] at full operating level**

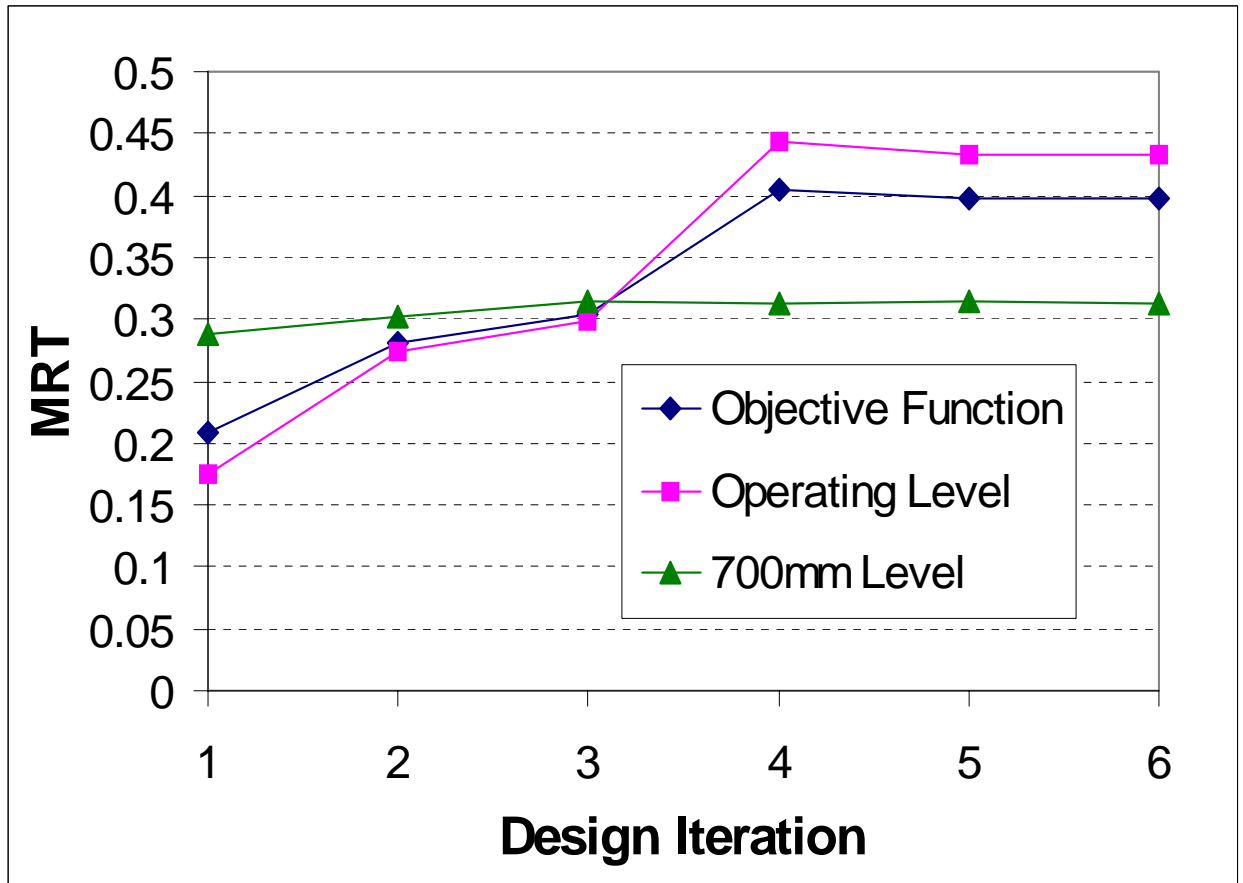
**( $x = (300,100,70,100,70,0)^T$ ) (Case 2)**

A validation study between on-site measurements (provided by ISCOR Vanderbijlpark) and the CFD modelling was also conducted to ensure the

validity of the CFD model. The results from this study are given in Appendix B.

### **4-3.3 Optimisation Results (DYNAMIC-Q)**

The results of the optimisation run obtained using the DYNAMIC-Q algorithm are given and discussed in this section. Figure 4-18 shows the optimisation history of the objective function as well as the MRT for operating level and at 700mm level. It can be seen that the objective function essentially levels out after 4 design iterations showing that the objective function has converged. The MRT for the operating level increased from 0.18 to 0.43 which represents an increase of 138%, while the MRT for the 700mm level increased from 0.29 to 0.31 which is an increase of 6.9%. The weighted combination of these two values (the objective function) can be seen to be dominated by the full operating level value. This relative insensitivity of the transition level MRT with respect to the design variables, is partly due to the fact that only 3 of the 6 variables influence the performance at the lower level, due to the fact that the upper hole in the baffle protrudes above the liquid steel at this level.



**Figure 4-18: Optimisation history of objective function (DYNAMIC-Q)  
(Case 2)**

Figure 4-19 shows the optimisation history of the design variables. An interesting fact to note is that the design variables are still changing after the 4<sup>th</sup> design iteration although the objective function has levelled off. This fact indicates that the last three designs in the optimisation run all have the same MRT although their geometries differ.

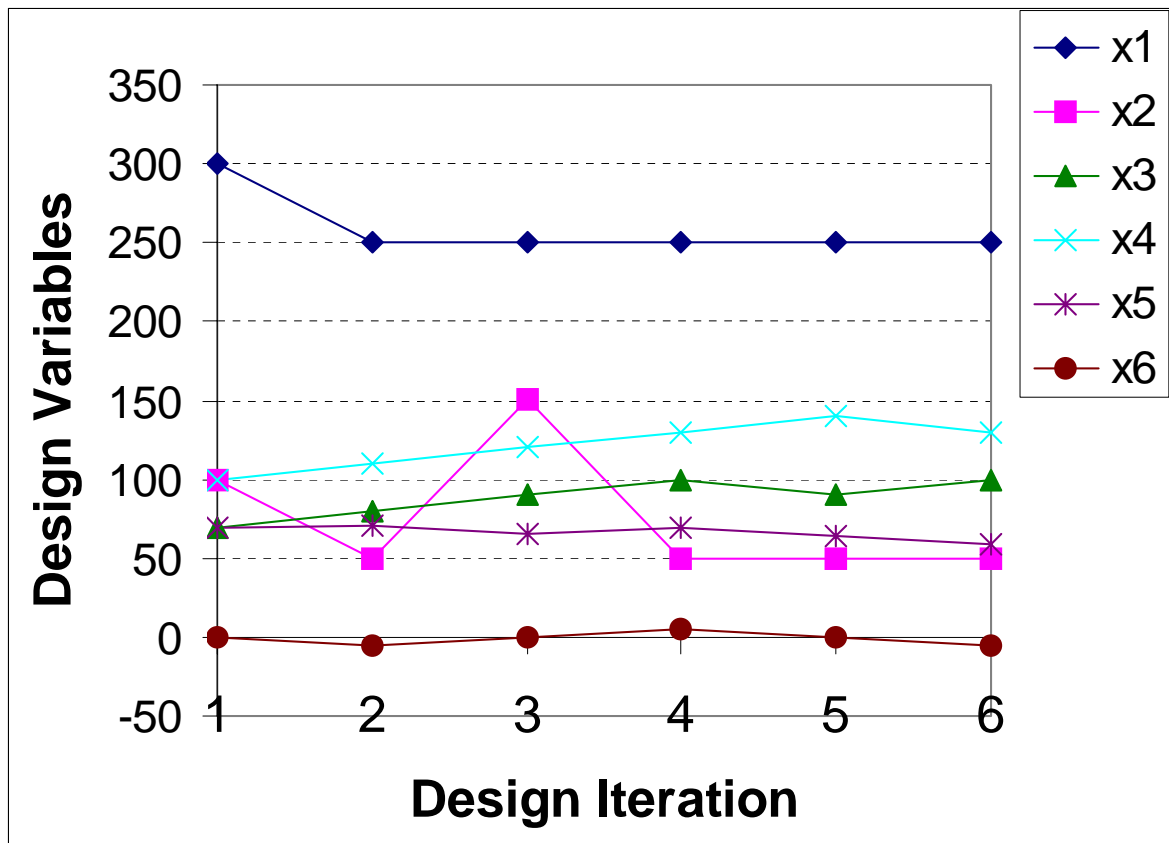


Figure 4-19: Optimisation history of design variables  
(DYNAMIC-Q) (Case 2)

Both the pouring box width ( $x_1$ ) and the baffle position ( $x_2$ ) converged to their respective allowable minimum values. The bottom hole diameter ( $x_3$ ) increased, while the top hole diameter ( $x_4$ ) and the top hole angle as seen from the side ( $x_5$ ) found a certain combination to establish a favourable flow pattern inside the tundish. The value of the top side hole angle as seen from the top ( $x_6$ ) oscillated around zero degrees, and the objective function seems to be relatively insensitive to this design variable.

#### 4-3.4 Optimisation Results (LS-OPT)

It can be seen that the objective function using LS-OPT essentially levels out after three design iterations showing that the objective function has converged (Figure 4-20). Due to the nature of the response surface approximation used in LS-OPT, it requires approximately 1.5 more simulations per optimisation iteration than DYNAMIC-Q. This implies that more or less the same number



of function evaluations (or CFD simulations) was performed for both DYNAMIC-Q and LS-OPT to achieve their respective optima.

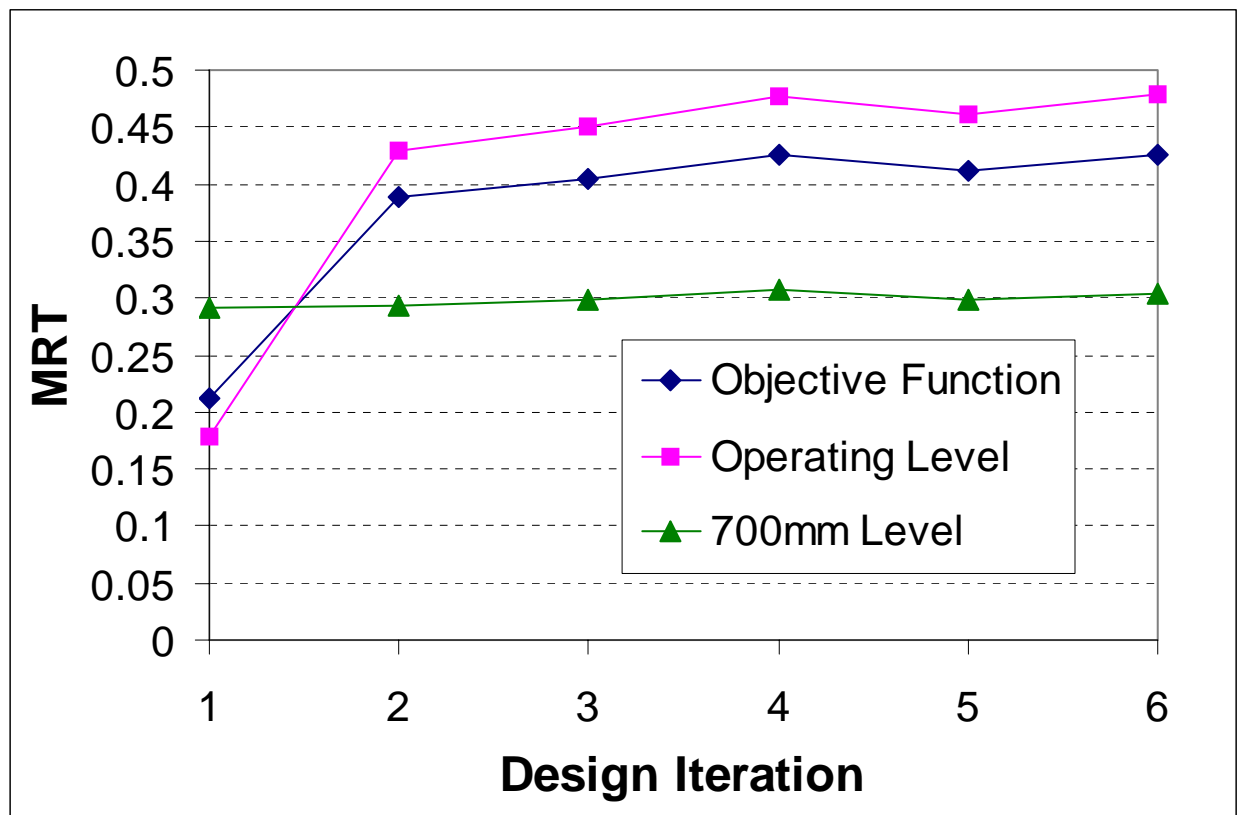
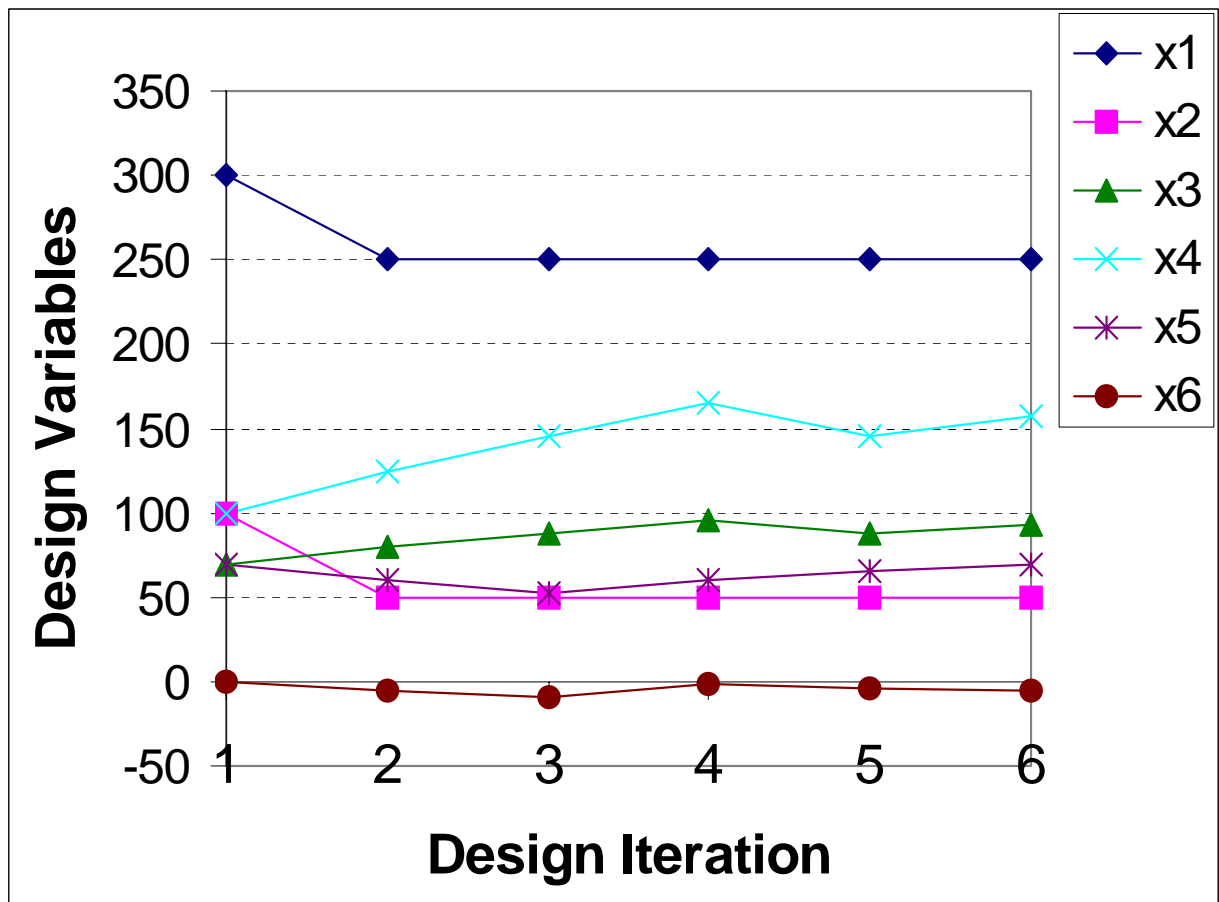


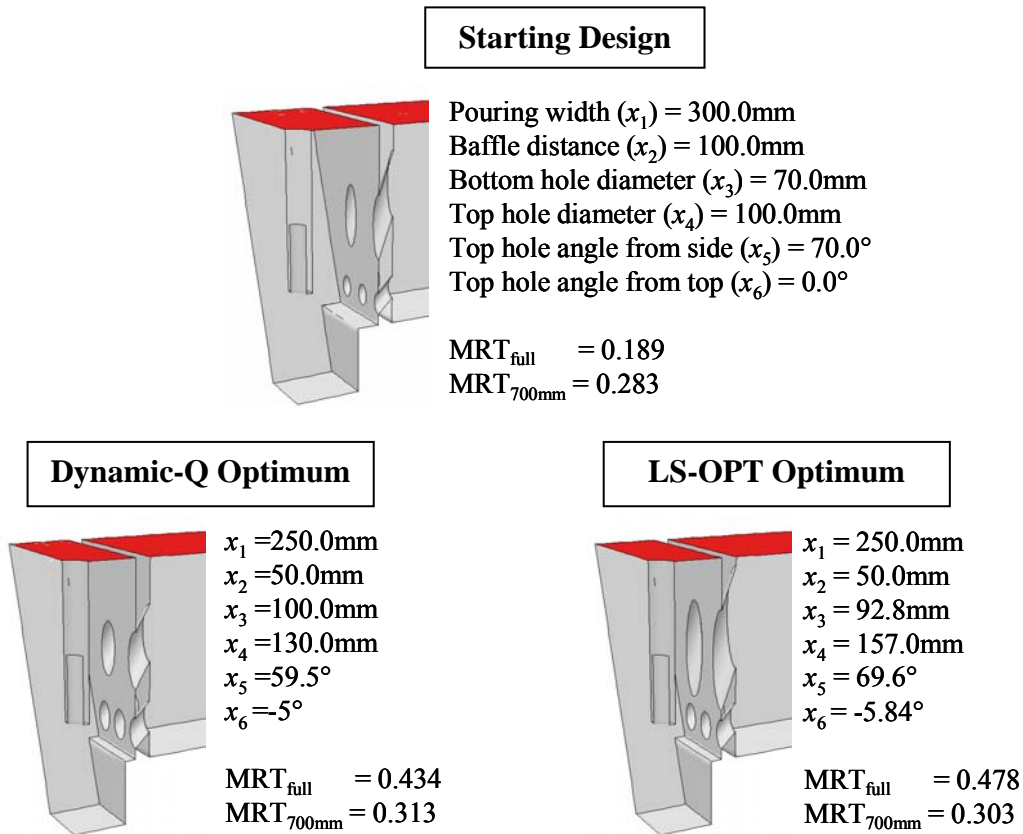
Figure 4-20: Optimisation history of objective function (LS-OPT) (Case 2)

The MRT for the operating level increased from 0.18 to 0.48, which represents an increase of 167%, while the MRT for the 700mm level again proved insensitive to the design changes. When using LS-OPT,  $x_3$ ,  $x_4$  and  $x_5$  converge to different values, while  $x_1$  and  $x_2$  again reached their respective minimum values (Figure 4-21).



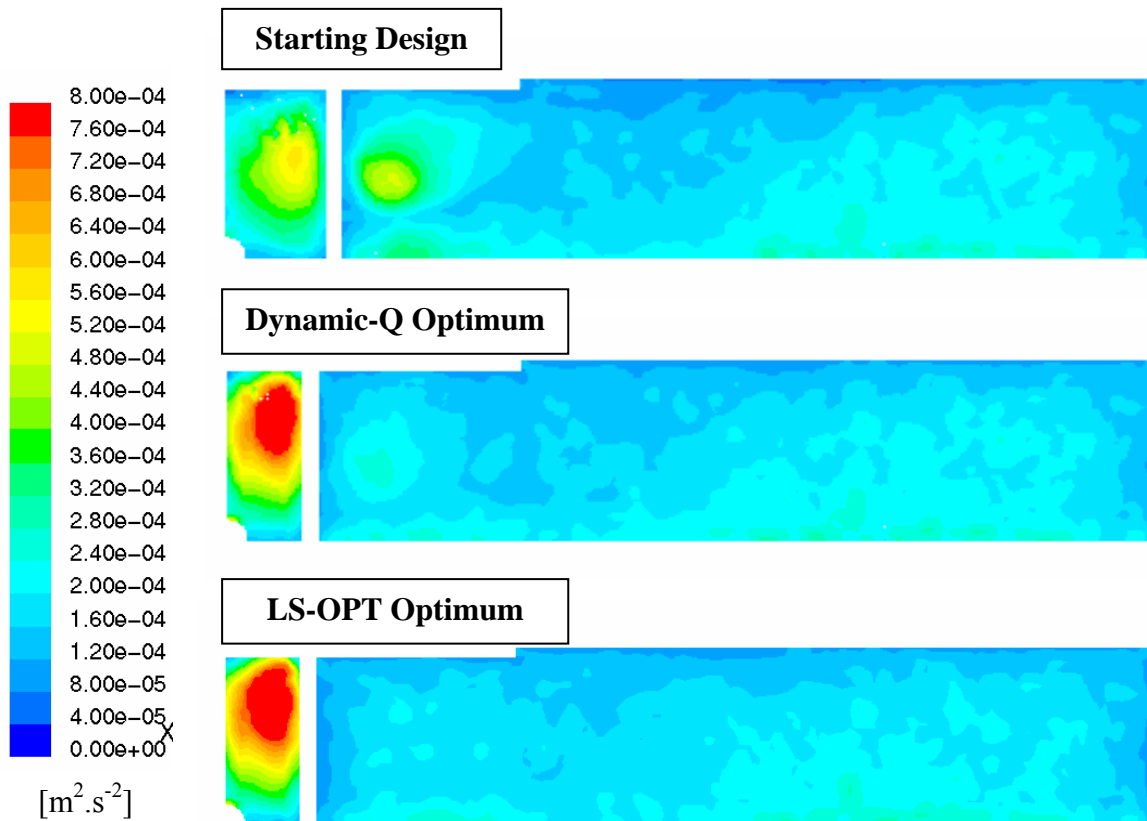
**Figure 4-21: Optimisation history of design variables (LS-OPT)  
(Case 2)**

The differences in the optimum design obtained by Dynamic-Q and LS-OPT are visually shown in Figure 4-22 together with the starting design. The difference between the MRT of the two optima obtained is mainly due to the top baffle hole diameter and angle. In the case of the optimum of DYNAMIC-Q, the top baffle hole diameter and angle is smaller than the optimum design obtained by LS-OPT. These smaller values have the effect of a higher velocity jet directed towards the outlet of the tundish. In turn, this has the effect that the MRT of the optimum obtained with DYNAMIC-Q is slightly less than that obtained with LS-OPT.



**Figure 4-22: Starting and final designs (DYNAMIC-Q and LS-OPT) (Case 2)**

A comparison of the surface Turbulent Kinetic Energy (TKE) for the starting design and the optima of Dynamic-Q and LS-OPT is given in Figure 4-23. The TKE for the two optima is higher than the starting design in the pouring box area, while the TKE downstream of the baffle is lower for the two optima.



**Figure 4-23: Comparison of turbulent kinetic energy on slag layer for the starting and final designs (DYNAMIC-Q and LS-OPT) (Case 2)**

#### **4-3.5 Conclusion**

This section showed the second case study where a commercial CFD package was combined with mathematical optimisation techniques to give optimum designs of tundish geometry and tundish furniture. The objective function used in this case was the maximisation of the MRT at operating and a typical transition level. The MRT was used as an indication of the cleanliness of the steel. The pouring box area and the baffle geometry were chosen as design variables in this case. FLUENT with its pre-processor GAMBIT was easily incorporated into an automatic loop for the optimisation. The two optimisation techniques used in this case study proved to be robust and economical. A 138% and a 167% improvement in the operating level MRT were obtained using the DYNAMIC-Q method and the LS-OPT method respectively.

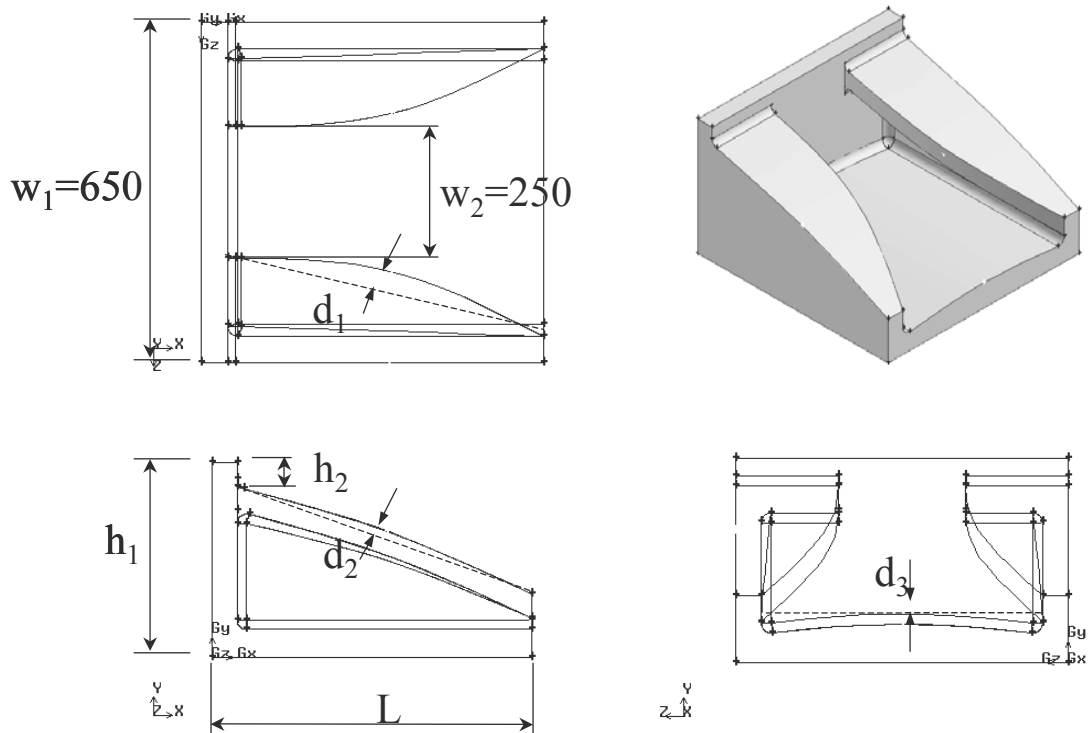
#### **4-4 CASE STUDY 3: IMPACT PAD OPTIMISATION**

The third case study is on a new impact pad design. Impact pads in tundishes have as their aim the reduction in the turbulence levels in the tundish. For this specific impact pad, the aim was to reduce the free-surface turbulence levels [74]. The design of the impact pad is also such that the flow is angled upwards toward the free-surface to improve the inclusion removal of the tundish. The impact pad is designed to be used in the single-strand stainless steel continuous caster in operation at the Middelburg plant of Columbus Stainless. This is the same tundish used in the first case study.

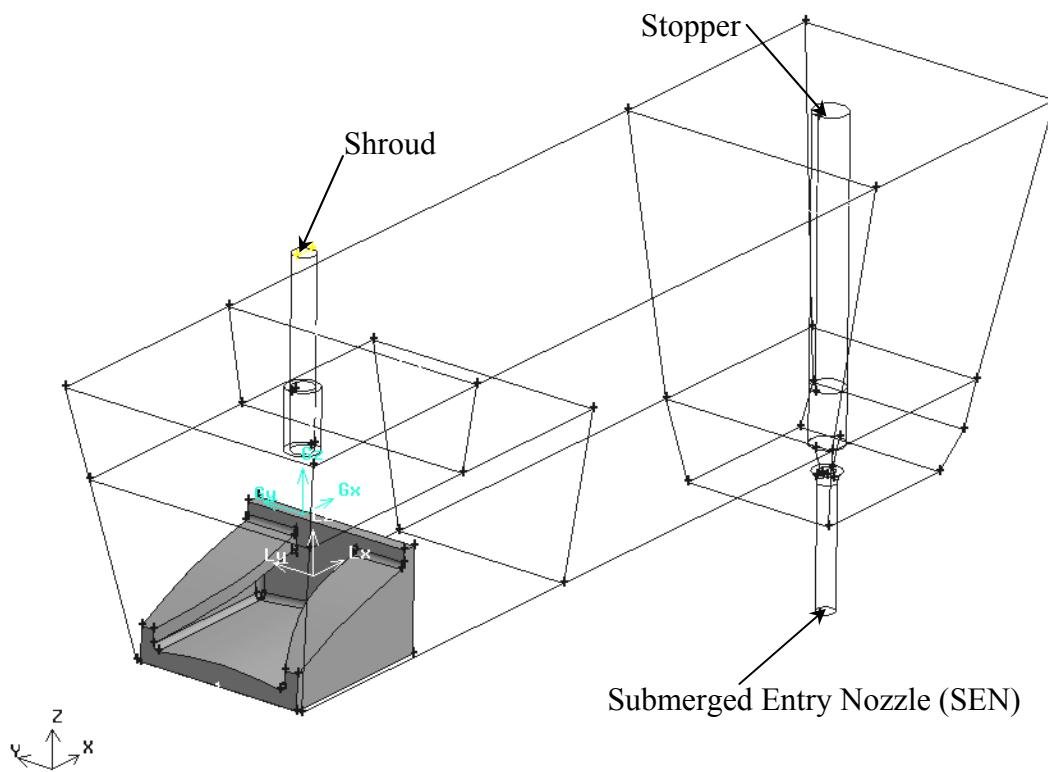
##### **4-4.1 Parameterisation of Geometry**

The impact pad geometry is shown Figure 4-24. The characteristics of the impact pad implies that it resorts under the Turbostop® [75] patent. The aim of the pad is to suppress turbulence through the creation of a recirculation zone within the pad through two overhead wings. As can be seen from the location of the impact pad in the tundish in Figure 4-25, the jet emanating from the shroud would impact the pad and then bend over on itself to flow towards the outlet. The pad has to suppress the turbulence of the jet so that it does not reach the surface above the pad with sufficient energy that could entrain slag. The lip on the pad has the function of angling the flow in the pouring box area upwards, much as a baffle with angled holes would do.

In order to optimise the impact pad, its geometry needs to be parameterised. The parameters chosen are shown in Figure 4-24. Initially, eight variables were chosen of which the values of two were fixed to the values shown in the figure. The value of  $w_1$  is assumed to be the full width of the tundish (refer Figure 4-25), while the value of  $w_2$  is such that the gap between the wings accommodates the possible motion of and uncertainty of the shroud position during casting. The three curvatures ( $d_1$  through  $d_3$ ) are parameterised as control points of Nonuniform Rational B-Splines (NURBS) used to define the geometry. A GAMBIT journal file that creates the impact pad given the of design variables and parameters is given in Appendix D.



**Figure 4-24: Schematic representation of impact pad with the design variables and fixed parameters (Case 3)**



**Figure 4-25: Graphical representation of impact pad inside tundish (Case 3)**

#### 4-4.2 Definition of Optimisation Problem

The complete mathematical formulation of the optimisation problem, in which the constraints are written in the standard form,  $g(\mathbf{x}) \leq 0$ , where  $\mathbf{x}$  denotes the vector of the design variables  $(x_1, x_2, x_3, x_4, x_5, x_6)^T = (L, h_1, h_2, d_1, d_2, d_3)^T$ , is as follows:

$$\begin{aligned} & \text{Minimize } [f(\mathbf{x}) = \max(\text{Turbulent kinetic energy on slag})], \\ & \text{subject to: } \begin{cases} g_j = -x_j + x_j^{\min} \leq 0; j = 1, 2, 3, \dots, 6 \\ g_{j+6} = x_j - x_j^{\max} \leq 0; j = 1, 2, 3, \dots, 6 \\ g_{13} = 200 - h_1 + h_2 \leq 0 \end{cases} \end{aligned} \quad (4-4)$$

where  $x_j^{\min}$  and  $x_j^{\max}$  are suitable minimum and maximum constraints for the  $j^{\text{th}}$ -component of the design vector,  $\mathbf{x}$ . The upper and lower bounds on the variables are given in Table 4-9 together with the initial subregion size as required by the optimiser. The last constraint in (4-4) is to prevent the fluid volume below the impact pad wings from collapsing.

**Table 4-9: Minimum, maximum and initial subregion of design variables (Case 3)**

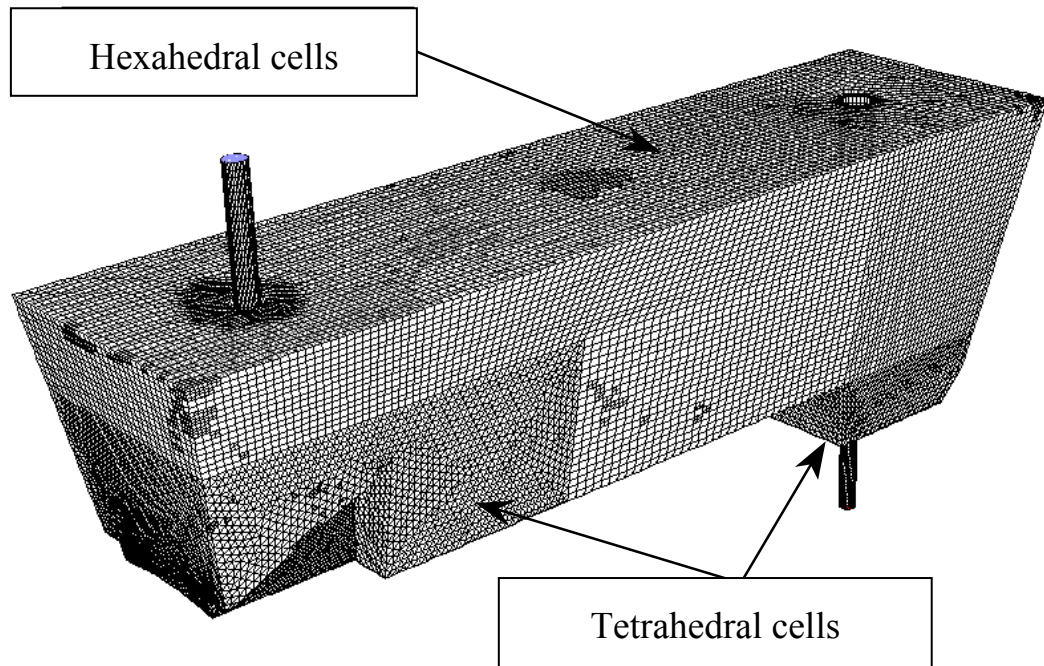
Variable	Minimum	Maximum	Initial subregion size
Length ( $L$ ) [mm]	400	1200	600
Total height ( $h_1$ ) [mm]	300	600	500
Lip height ( $h_2$ ) [mm]	40	N/A	20
Wing curvature ( $d_1$ ) [mm]	0	100	50
Side curvature ( $d_2$ ) [mm]	0	100	20
Floor curvature ( $d_3$ ) [mm]	0	40	10

#### 4-4.3 CFD Modelling

##### Grid Generation and Model Set-up

A typical grid of the tundish is shown in Figure 4-26. The grids used in the optimisation contained in the order of 400 000 cells after grid adaption. It can

be seen in Figure 4-26 that most of the tundish contains hexahedral cells while the complex regions (i.e., around the impact pad and at the bottom of the stopper) contain tetrahedral cells. Due to the off-set of the shroud, the model had no symmetry that could be used to reduce the computation domain.



**Figure 4-26: Typical grid of tundish with impact pad (Case 3)**

#### Boundary Conditions and Fluid Properties

The boundary conditions used are shown in Figure 4-27. The heat fluxes were derived from on-site temperature measurements provided by Columbus Stainless. The fluid and thermal properties of the steel used are given in Table 4-10.



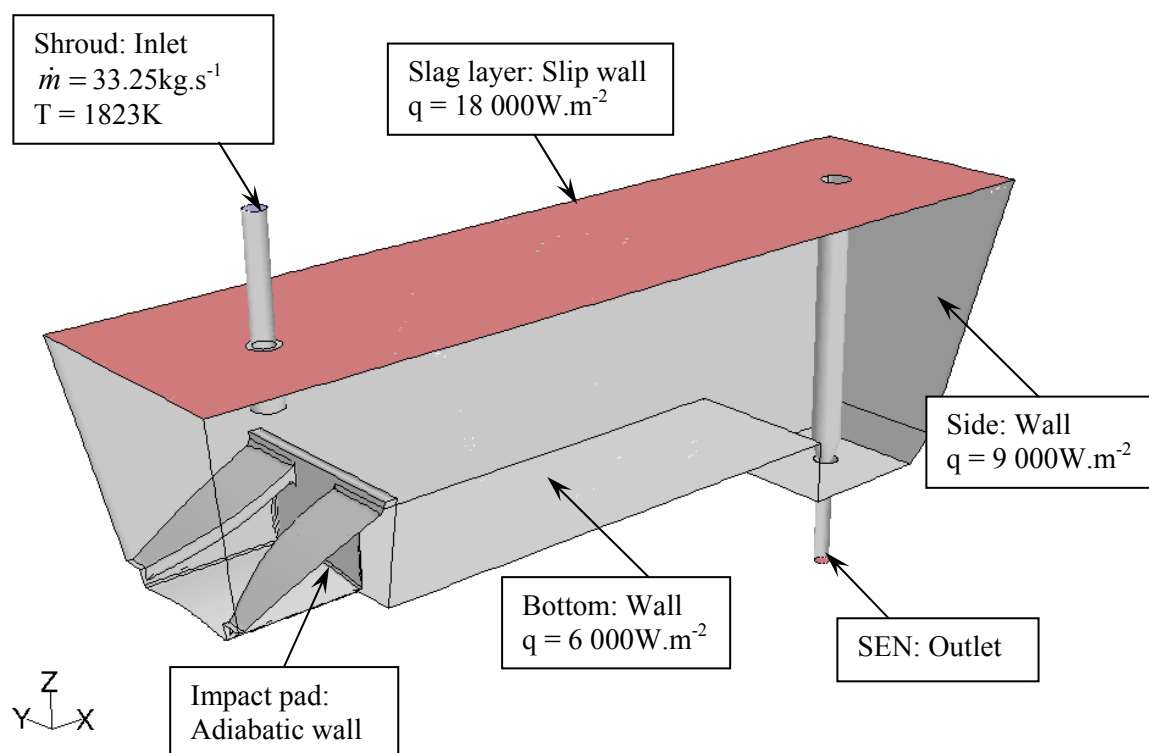


Figure 4-27: Boundary conditions (Case 3)

Table 4-10: Fluid and thermal properties of steel used for Case 3

Property	Value
Thermal expansion coefficient	$0.1107 \times 10^{-3}$
Reference density [ $\text{kg.m}^{-3}$ ]	6975
Reference temperature [K]	1773
Specific heat of liquid steel [ $\text{J.kg}^{-1}.\text{K}^{-1}$ ]	817.3
Conductivity of liquid steel [ $\text{W.m}^{-1}.\text{K}^{-1}$ ]	31.0
Dynamic viscosity of liquid steel [Pa.s]	0.0064

#### Computational Implementation and Run-Time

As mentioned above, the commercial CFD code, FLUENT is used in this case study. For the simulations presented in this case, the Reynolds-Averaged Navier-Stokes equations are solved with the  $k-\epsilon$  turbulence model providing the turbulent closure. Second-order discretisation is used for all the flow equations while a three-order drop in the sum of the scaled residuals was considered to constitute a converged solution. The CFD model was run in parallel on three Pentium 4 1.7GHz machines operating under RedHat Linux

Version 7.2 . In this mode, each steady-state CFD simulation had a run-time of approximately 6 hours. Due to the 50% over-sampling used in the  $D$ -optimality implementation in LS-OPT, each optimisation iteration required  $N=11$  experimental designs or CFD simulations, implying 66 hours per optimisation iteration.

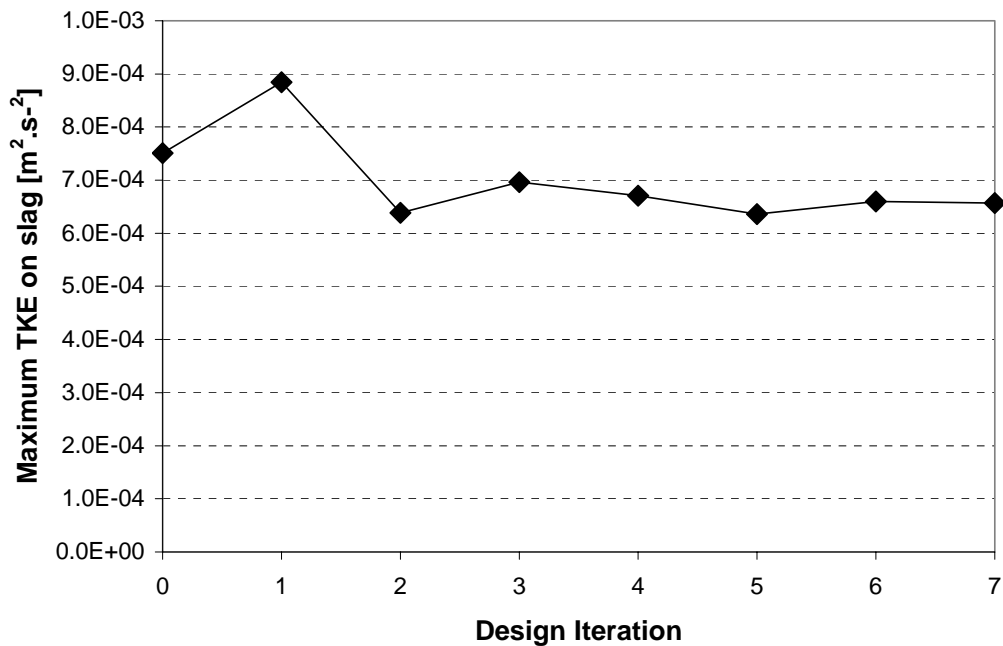
The set-up and solution procedure in FLUENT was automated by using a FLUENT journal file and is given in Appendix E. This journal file writes the appropriate files to the computer's hard disk. The Fortran programs given in Appendix F are used to extract the appropriate data from these files that is to be used by the optimiser.

#### **4-4.4 Optimisation Results**

The optimisation results presented here are firstly the optimisation history of the objective function defined in (4-4), and then the optimisation history of the six design variables,  $x$ . In addition, some functions were monitored during the optimisation process. These include inclusion particle statistics, yield information and impact pad volume.

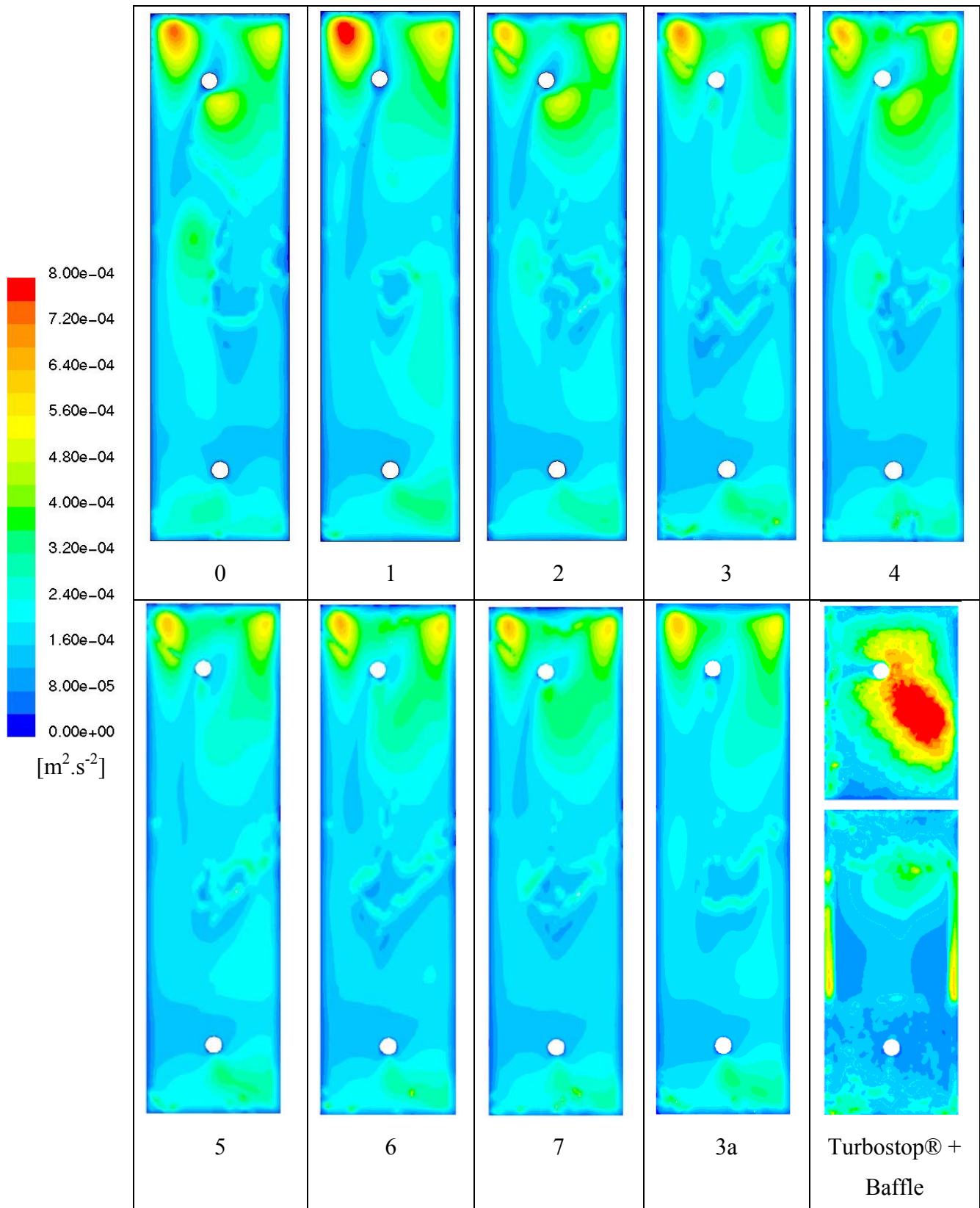
##### Objective Function

The optimisation history for the objective function defined in (4-4) is shown in Figure 4-28. The improvement obtained is not very significant (12.5% improvement compared to the starting design), mainly due to the fact that the chosen initial design had a fairly low TKE so start with.



**Figure 4-28: Optimisation history of objective function (Case 3)**

As the objective function only represents the maximum TKE value on the slag surface, it is of interest to see how its reduction influences the distribution of TKE on the whole slag layer. This can be seen in Figure 4-29, where the TKE contours on the slag layer are shown for the different designs obtained during the optimisation history. All the contours range between 0 and  $8\text{e-}4 \text{ m}^2 \cdot \text{s}^{-2}$ . The surface TKE for the tundish with Turbostop<sup>®</sup> and baffle [76] is shown for comparison. It can be seen that that design had much higher TKE values than the current design. The higher TKE levels can be due to the fact that the Turbostop<sup>®</sup> is not optimised for the specific tundish configuration or the presence of the baffle. Note how the size of the maximum contour level in TKE is reduced by the optimiser for the current impact pad. Also shown in Figure 4-29, is design 3a that represents design iteration 3 where the values of the design variables were rounded to the nearest millimetre for manufacturing purposes.



**Figure 4-29: Turbulent kinetic energy on slag layer for different designs in optimisation history compared to the Turbostop™ and baffle configuration (Case 3)**

Design Variables

The history of the design variables is shown in Figure 4-30. The two height variables exhibit the largest change during the optimisation. The physical influence of these variables on the geometry can be seen more clearly in Figure 4-31 where isometric views of the impact pads of which the TKE contours were shown in Figure 4-29, are displayed. The most notable difference in the optimum design from that of the baseline, is an overall reduction in height ( $h_1$ ) with an increase in the lip height ( $h_2$ ). Although the length of the impact pad ( $L$ ) was not constrained, the optimiser did not attempt to increase its length. In fact, the length was reduced slightly. The maximum TKE proved relatively insensitive to the three curvatures ( $d_1$ ,  $d_2$ , and  $d_3$ ). Both the wing and floor curvatures increased slightly, while the side curvature remained constant.

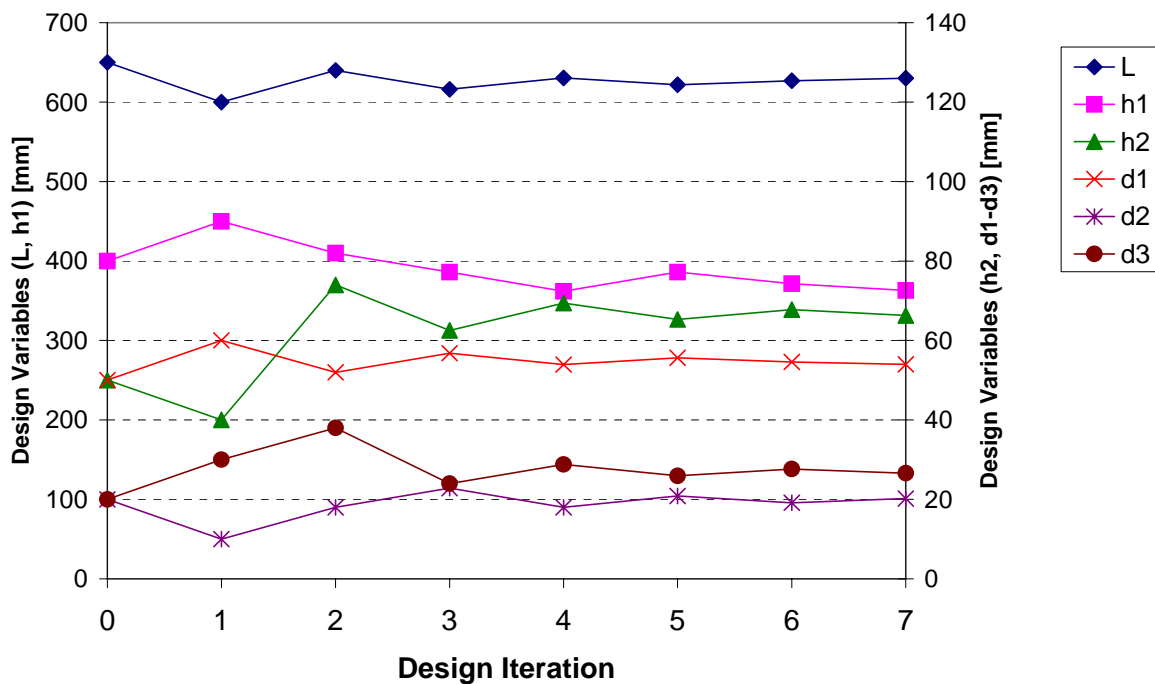
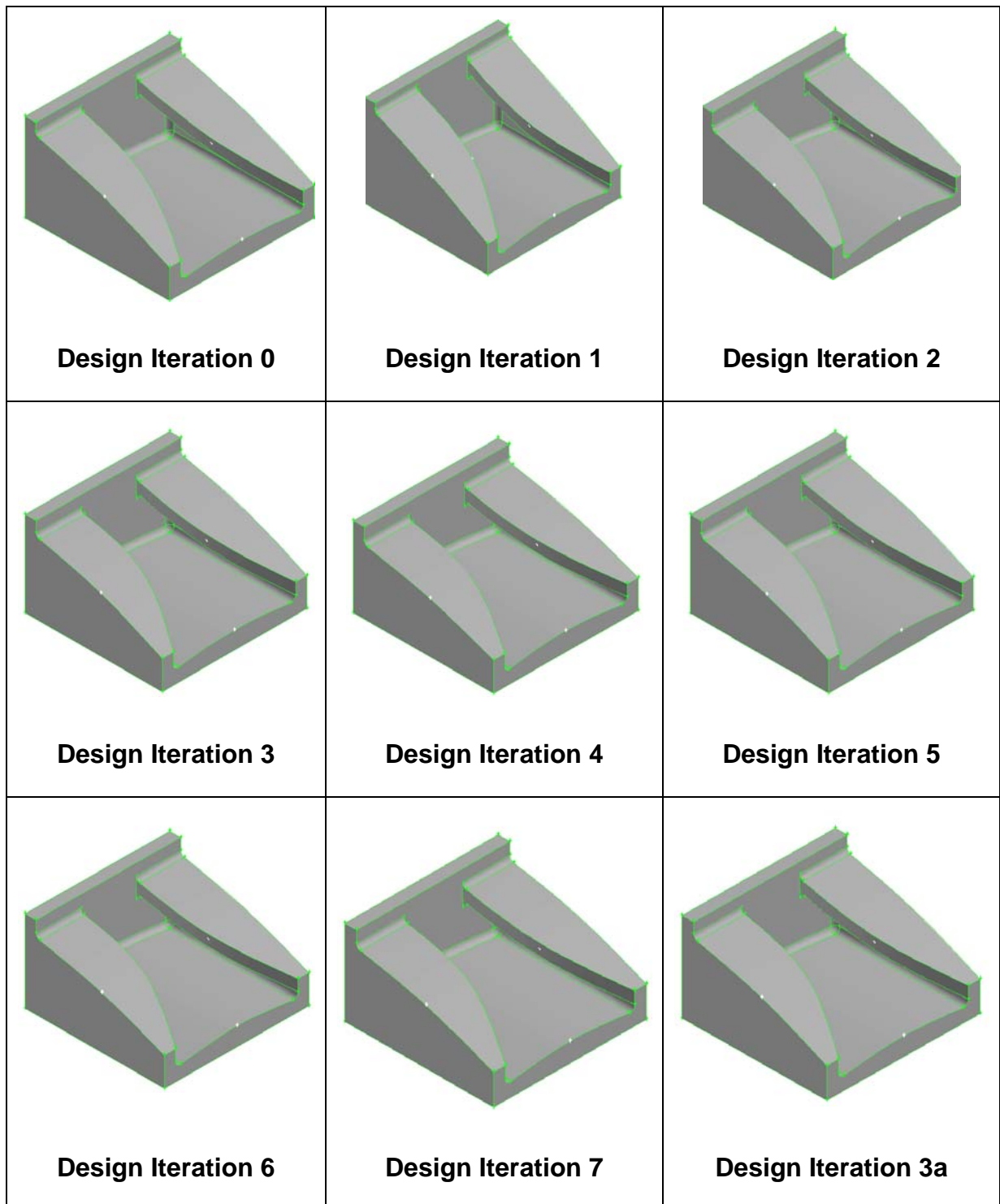


Figure 4-30: Optimisation history of design variables (Case 3)

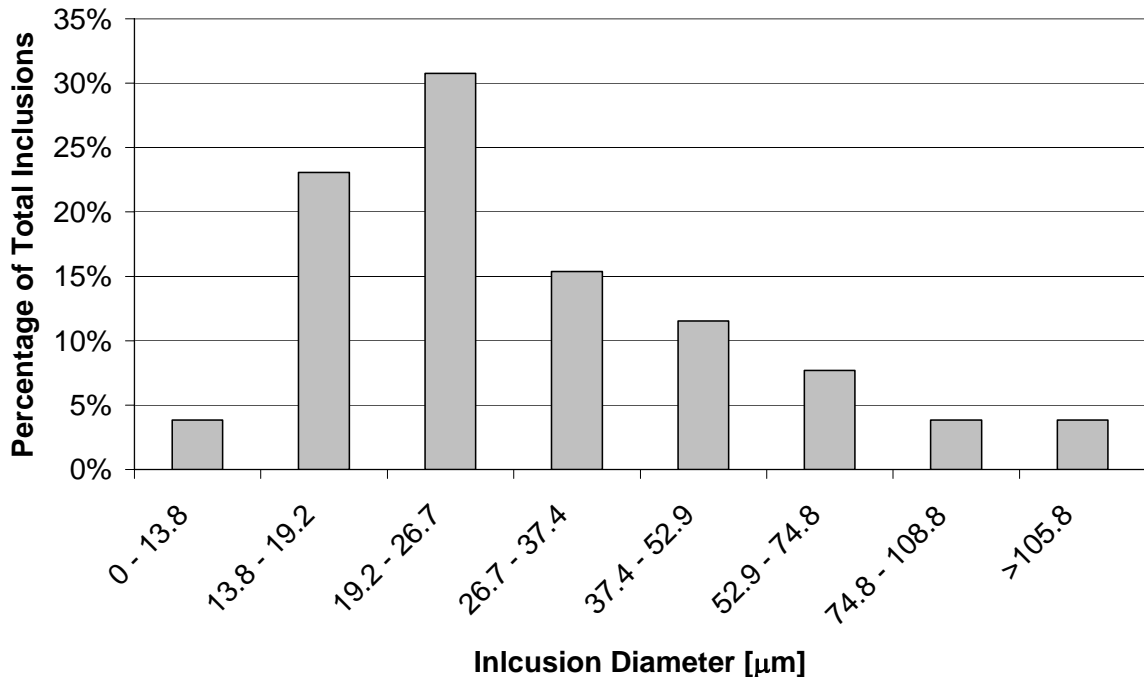


**Figure 4-31: Optimisation history of design (Case 3)**

Monitored Functions

Although not included in the design optimisation process, three other possible design criteria were monitored. Firstly, the inclusion particle removal capability due to the impact pad design was monitored. A typical size

distribution obtained from on-site sampling of the steel in the ladle (provided by Columbus Stainless), as shown in Figure 4-32, was introduced into the inlet to the tundish.



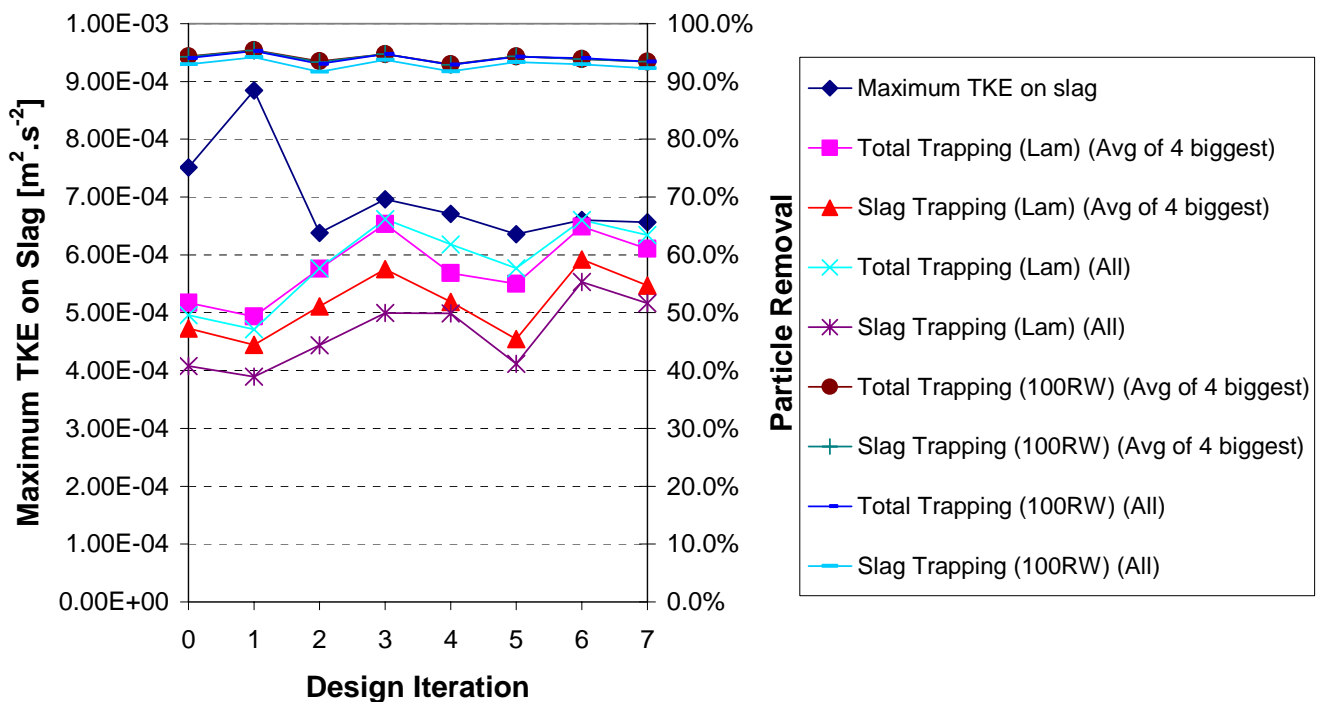
**Figure 4-32: Size distribution of inclusion at inlet of tundish (Case 3)**

Figure 4-33 shows the particle removal on the slag layer during the optimisation process using the Lagrangian tracking method explained in section 2-2.4.4 as available in FLUENT. Two methods for the particle tracking are investigated. The first is without the effects of the turbulence on the particle trajectory, indicated by the abbreviation *Lam* in brackets in Figure 4-33. The second is including the effect of turbulence using 100 stochastic tracks for each release point as explained in 2-2.4.4, indicated by the abbreviation *100RW* in brackets in Figure 4-33.

The removal efficiencies for the above two mentioned methods are shown for the larger particles as well as for all the particles size combined. Interestingly, note how the particle removal trend is initially opposite to that of turbulence suppression, but from the third iteration onwards, a reduction in turbulence

levels on the slag surface (as quantified by TKE) corresponds to fewer particles being trapped on the slag layer. The trapping of the four largest particle groups considered (all larger than  $37\mu\text{m}$ ) correlate with the trapping of all the particle sizes modelled.

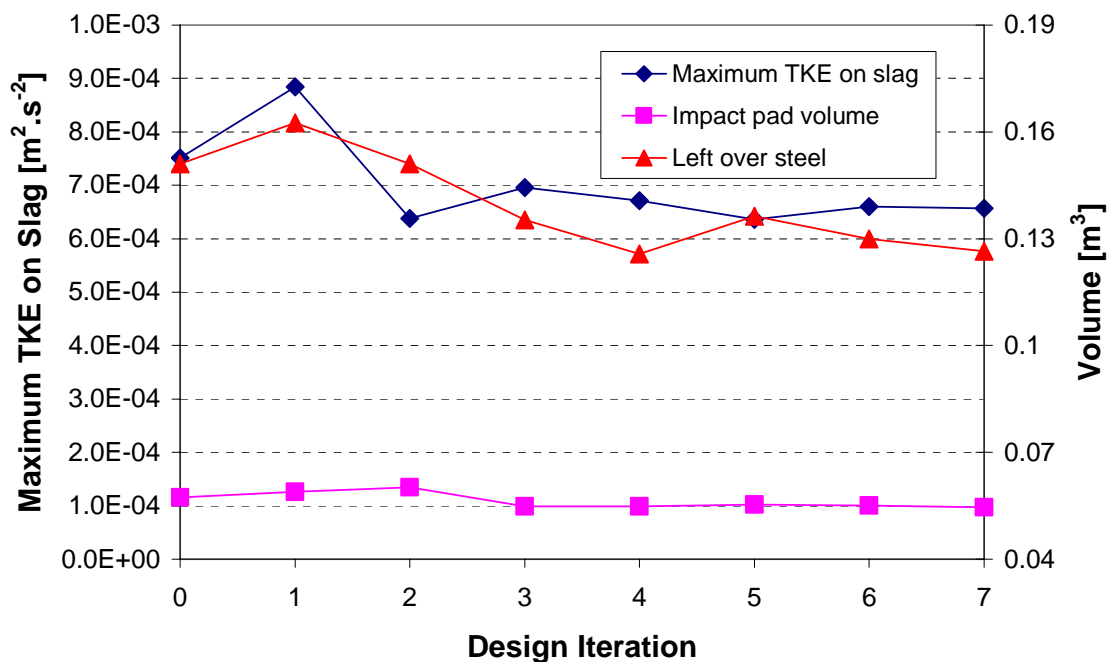
The particle tracking without including the effect of turbulence on the particle trajectory is consistently lower than the case where turbulence is considered. This can be explained as follows. For the case without turbulence effects, the particles get close to the slag surface due to the nature of the flow in the tundish, but tend to travel along the surface without touching the surface as the buoyancy forces are too small to let the particles float to the top. For the case where turbulence is considered in the particle trajectory calculation, the particles also tend to get close to the slag surface but due to the nature of the stochastic tracking model, the particles are perturbed due to the effect of turbulence, causing them to touch the slag layer in more instances.



**Figure 4-33: Optimisation history of monitoring functions (particle removal) (Case 3)**



The second and third functions that were monitored to assist in the evaluation of the design are the impact pad volume (as a measure of its cost and weight for handling purposes) and the volume of steel remaining in the tundish behind the impact pad after draining. These two functions are given in Figure 4-34 together with the objective function. Although not expected because these functions were not explicitly used in the optimisation formulation, both these quantities were reduced as the objective was minimised.



**Figure 4-34: Optimisation history of monitoring functions (volumes)  
(Case 3)**

The numerical values of the objective and monitored functions are given in Table 4-11 for direct comparison. Again design 3a represents design iteration 3 where the values of the design variables were rounded to the nearest millimetre for manufacturing purposes. The details are discussed in 4-4.5 below.

**Table 4-11: Optimisation history of objective and selected monitoring functions (Case 3)**

Iteration	Maximum k on slag [m <sup>2</sup> .s <sup>-2</sup> ]	Total trapping percentage (Laminar) Avg of 4 largest)	Total trapping percentage (100RW) Avg of 4 largest)	Volume steel left over [m <sup>3</sup> ]	Impact pad volume [m <sup>3</sup> ]
0	0.000751	47.25%	94.25%	0.15098	0.05734
1	0.000884	44.42%	95.35%	0.16255	0.05888
2	0.000638	51.09%	93.36%	0.15100	0.06020
3	0.000696	57.55%	94.71%	0.13530	0.05476
4	0.000671	51.89%	92.86%	0.12576	0.05481
5	0.000636	45.41%	94.30%	0.13638	0.05538
6	0.000660	59.20%	93.84%	0.13001	0.05503
7	0.000657	54.72%	93.39%	0.12647	0.05458
3a	0.000640	55.25%	94.88%	0.13464	0.05457

#### **4-4.5 Chosen design**

In an attempt to present a compromised design, the design in iteration 3 was chosen for manufacture. This is because its maximum TKE is reasonable, but more importantly it had the highest particle removal rate of the first five designs (those available when the design was frozen). The variables describing the geometry of Iteration 3 were rounded to values as would be required for the manufacture of the impact pad. The performance parameters (TKE and particle removal statistics) for this design were included in the results above (See 3a in Figure 4-29 and Figure 4-31). As can be seen in Table 4-11, the modified design 3a outperforms design 3, in that it has a lower maximum TKE, and similar particle removal. The values of the rounded variables are given in Table 4-12.

**Table 4-12: Rounded variable values – Design 3a (Case 3)**

Variable	Value
Length ( $L$ ) [mm]	615.0
Total height ( $h_1$ ) [mm]	385.0
Lip height ( $h_2$ ) [mm]	60.0
Wing curvature ( $d_1$ ) [mm]	56.0
Side curvature ( $d_2$ ) [mm]	20.0
Floor curvature ( $d_3$ ) [mm]	24.0

#### **4-4.5.1 Flow Results of Chosen Design**

In addition to the optimisation results of design 3a given above, Residence Time Distribution (RTD) results are given in this section. Detailed steady flow results are given in Appendix G. These results are to serve as comparison to that of other previous and future designs as well as with water model results.

##### RTD data of chosen design

A transient simulation of the chosen was performed. This simulation took the form of monitoring the outlet concentration for a step input of tracer at the inlet. The resulting distribution was differentiated numerically to obtain the familiar RTD curve. The typical RTD related quantities were calculated and are given in Table 4-13. The values obtained with this impact pad are again compared to that of the Turbostop® and baffle configuration calculated in a previous study [76]. The dead volume in the tundish has increased to nearly 40% compared to the 26% of the original Turbostop® and baffle (also in Table 4-13). This result emphasises the need for a well-designed dam near the outlet to not only prevent short-circuiting, but to also reduce the dead zones in the tundish.

**Table 4-13: RTD-related data (Case 3)**

Quantity	Impact pad	Turbostop® + baffle [76]
Theoretical Mean Residence Time, $\bar{t}$	679.9 s	669.8 s
Tundish volume	3.241 m <sup>3</sup>	3.193 m <sup>3</sup>
Dispersed Plug Flow Volume	19.4%	23.6 %
Mixed Flow Volume	41.1%	50.4 %
Dead Volume	39.5%	25.9 %
Minimum Residence Time (MRT)	0.170	0.192
Peak Residence Time (PRT)	0.216	0.281
Actual mean residence time ( $\theta_{mean}$ )	0.605	0.741

#### **4-4.6 Water Model and Plant Implementation**

The optimised impact pad was manufactured and tested in the tundish water model at the University of Pretoria [77]. Visual observations of the water model were made with respect to surface appearance and dye flow patterns as detailed in the technical note [78]. A summary of the observations of water model with the impact pad as compared to an empty tundish is given in Table 4-14.

**Table 4-14: Visual observation of surface and dye flow patterns [78]**

Configuration	Visual observation
New impact pad design	Quiet surface appearance around inlet stream Slight movement visible along the back wall (wall furthest from outlet) area No stagnant zones visible
Empty tundish	Quiet surface appearance Short circuiting of dye to outlet stream No stagnant zones visible.

The optimised impact pad was also manufactured for plant trials at Columbus Stainless, where it underwent extensive plant trials [79,80]. The initial trials

[79] indicated that the 304 stainless steel grade showed a reduction in defects with the new impact pad compared to the case without any furniture. The 409 stainless steel grade however showed an increase in the number of defects when using the new impact pad compared to Columbus Stainless' current furniture. The results from the initial trial motivated a long-term trial for the new impact pad [80]. The long-term trial indicated that the impact pad decreased the defects in the austenitic material (e.g., 304, 316), while increasing the defects in the ferritic material (e.g, 409). From this, it was recommended that the new impact pad should be implemented on a long-term basis on the 304 steel grade. The difference in performance for the ferritic and austenitic material in the plant trials highlighted the current challenge for CFD to model the detailed metallurgical reactions that occur in different steel grades (e.g., inclusion formation and the interaction with the slag layer) to explain why there is difference in the impact pad performance of these two grades.

#### **4-4.7 Conclusions**

This section described the optimisation of an impact pad for the single-strand tundish of Columbus Stainless. The techniques of CFD coupled with mathematical optimisation were used in the form of the commercial solver FLUENT, its pre-processor GAMBIT and the commercial optimiser, LS-OPT. The objective function used was the maximum turbulent kinetic energy on the slag surface. Six design variables describing the impact pad geometry were used. A 12.5% reduction in maximum surface turbulent kinetic energy was obtained during the optimisation. During the optimisation process, the inclusion particle removal capability of the design was monitored as well as impact pad volume and liquid steel yield.

## 4-5 CASE STUDY 4: DAM OPTIMISATION WITH IMPACT PAD

In the last test case, a dam was introduced in the tundish combined with the previously optimised impact pad. This introduction of the dam was an attempt to deflect the flow upwards in order to remove inclusions by trapping them on the slag layer without affecting the turbulence suppressing capability of the tundish with impact pad.

### 4-5.1 Parameterisation of Geometry

The chosen design (design 3a) of the impact pad of Case Study 3 was kept fixed, while the dam introduced two additional variables, i.e., the height of the dam ( $p_1$ ), and the position of the dam from the left corner of the tundish ( $h_3$ ), as shown in Figure 4-35.

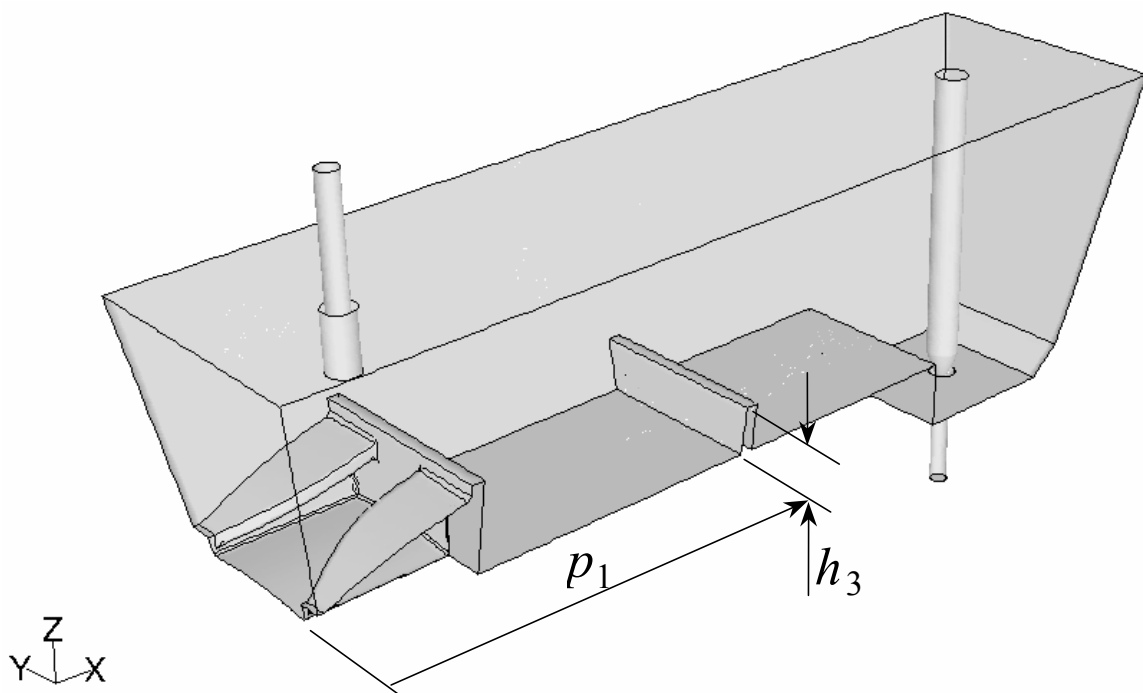


Figure 4-35: Design variables of dam (Case 4)

### 4-5.2 Definition of Optimisation Problem

In this case study, the inclusion removal on the slag layer was maximised. The inclusion particles were assumed to be trapped by the slag layer when they came in contact with the slag layer. The definition of the optimisation problem in the standard form is given in equation (4-5) where  $\mathbf{x}$  denotes the vector of design variables  $(x_1, x_2)^T = (p_1, h_3)^T$ .

$$\begin{aligned} & \text{Maximise } [f(\mathbf{x}) = \text{Particle Trapping}(\mathbf{x})] \\ & \text{subject to: } \begin{cases} g_j = -x_j + x_j^{\min} \leq 0; j = 1, 2 \\ g_{j+2} = x_j - x_j^{\max} \leq 0; j = 1, 2 \end{cases} \end{aligned} \quad (4-5)$$

The minimum and maximum allowable values for the optimisation problem are given in Table 4-15 together with the initial subregion size required by LS-OPT. The minimum and maximum values were chosen purely from a geometrical constraint, i.e., the values were chosen so that the dam would fit into the tundish and that there is space between the top of the dam and the slag layer to allow the steel to flow over the dam.

**Table 4-15: Minimum, maximum and initial subregion of design variables (Case 4)**

Variable	Minimum	Maximum	Initial subregion size
Position of dam ( $p_1$ ) [mm]	1500	2700	1000
Height of dam ( $h_3$ ) [mm]	50	750	400

### 4-5.3 Inclusion Particle Modelling Approach

In this case study the Lagrangian particle tracking method, as described in section 2-2.4.4, is used. The effect of turbulence on the inclusion removal is included by using the stochastic tracking method discussed in the same section. 100 stochastic tracks for each injection point are used and the same inclusion size distribution as in the third case study is used as given in Figure 4-32.

Particles touching the sides and bottom of the tundish and the tundish furniture are assumed to be reflected back into the molten steel flow.

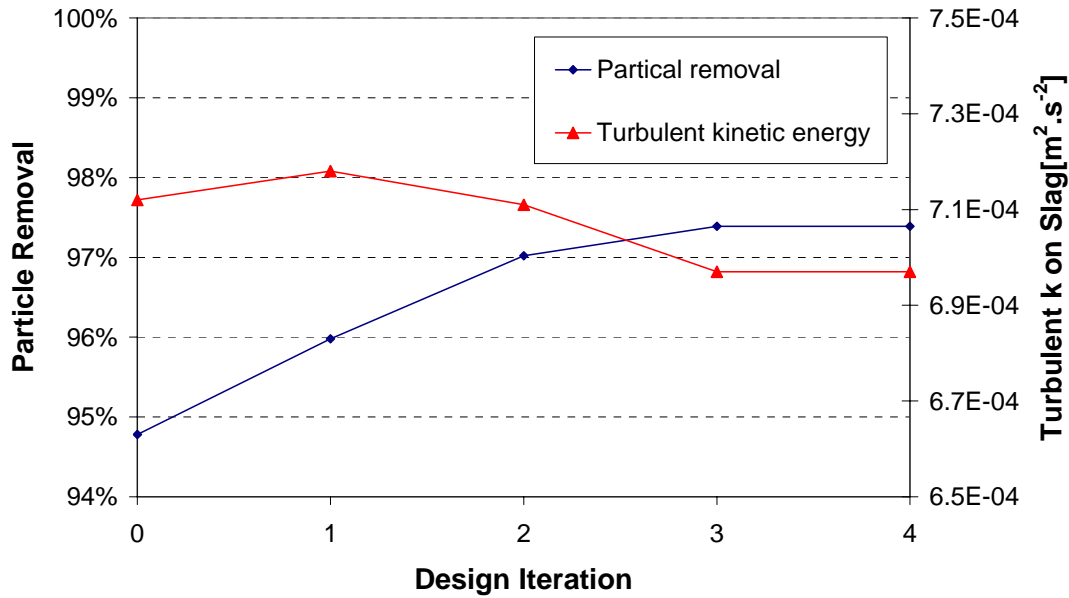
#### **4-5.4 Optimisation Results**

##### *Objective function and monitoring function*

The history of the objective and monitored function is given in Figure 4-36. As shown, the particle removal increased from just under 95% removal to above 97% removal by the slag layer. Although the maximum turbulent kinetic energy on the slag layer did not form part of the optimisation problem, it was monitored to see what the effect of the introduction of the dam would have on the turbulence of the slag surface. In this case, the maximum turbulent kinetic energy proved to be insensitive to the introduction of the dam and the optimised case even had a slightly lower value. This can be explained by the fact that the maximum values on the slag surface occur close to the shroud and the dam does not introduce higher levels of turbulence in the slow-moving liquid in the area of the dam.

If it were found that the turbulent kinetic energy was higher than the starting design, it could explicitly form part of the optimisation through the introduction of a constraint function limiting the maximum turbulent kinetic energy on the slag layer to be below the value of the case without a dam.

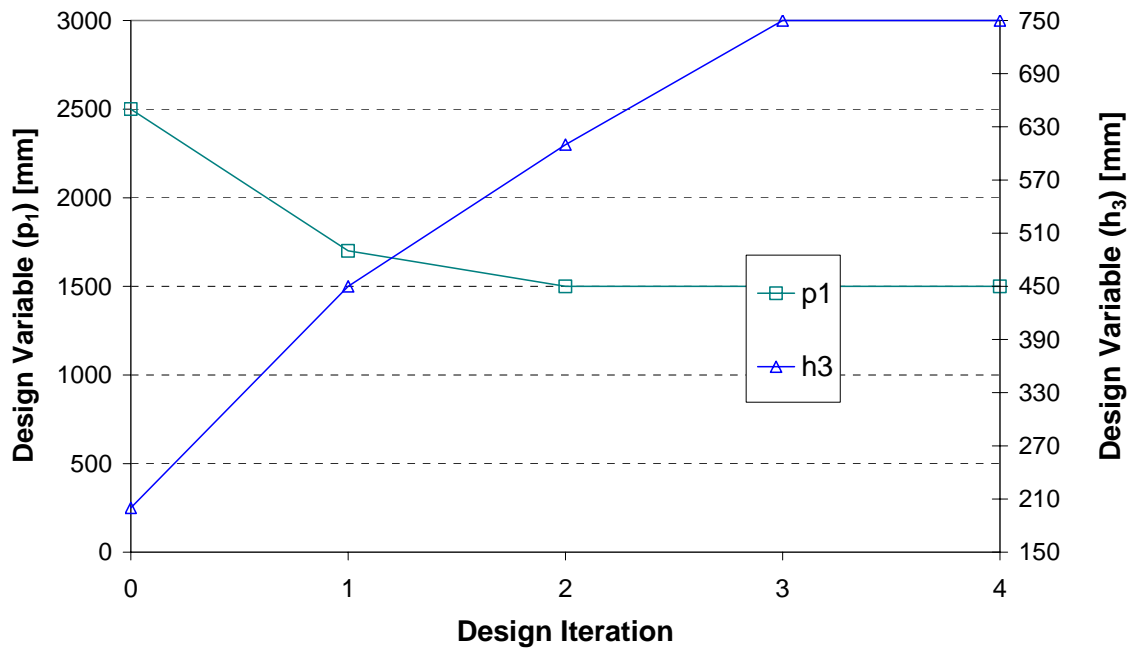




**Figure 4-36: Optimisation history of objective function (Case 4)**

#### Design Variables

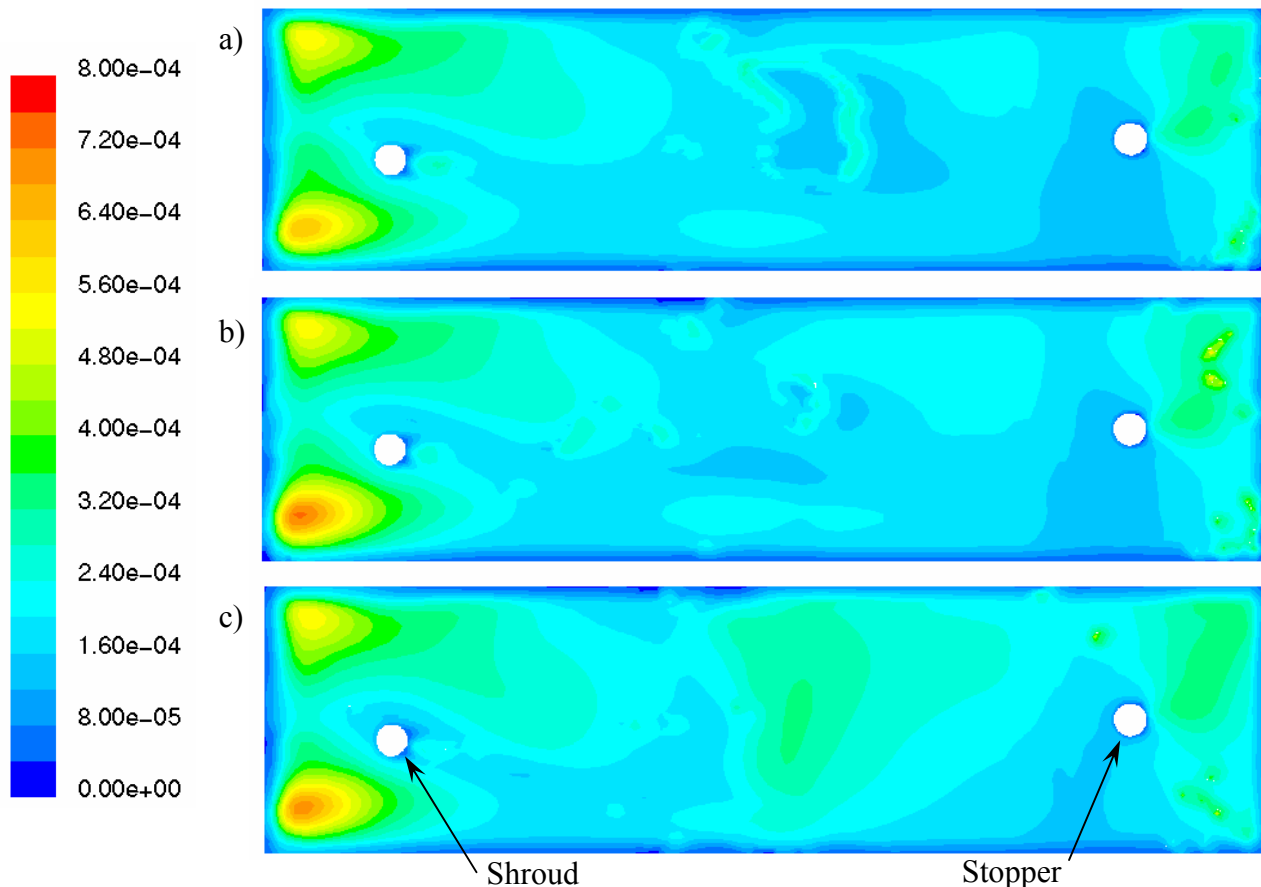
The history of the design variables is shown in Figure 4-37. As can be seen in this figure, the optimum dam configuration for particle removal is the highest allowable dam as close to the shroud as allowed. The result makes intuitive sense as the flow is deflected upwards and the chance of a particle reaching the slag layer is improved. This optimum design is however impractical looking at it from a yield prospective unless draining holes are inserted into the dam. This shows how important the initial formulation of the optimisation problem is. The yield can also form part of the optimisation problem as a constraint and then the optimiser will find an optimum within the prescribed yield limit.



**Figure 4-37: Optimisation history of design variables (Case 4)**

#### **4-5.5 Flow Results**

An important aspect of introducing a dam, is that the dam should not increase the surface turbulent kinetic energy. The turbulent kinetic energy for the case without the dam, with the initial design dam, and the optimised dam are shown in Figure 4-38. The higher turbulence levels that are introduced by the dam can be seen by the higher (more green) contours present in the centre of the slag layer shown in Figure 4-38c). These higher turbulence levels are still lower than the maximum values that occur near the shroud.



**Figure 4-38: Turbulent kinetic energy without dam (a) and with initial dam (b) and with optimised dam (c) (Case 4)**

#### **4-5.6 Conclusion**

A dam was used in conjunction with the optimised impact pad of case study 3. The position and height of the dam were optimised to give the maximum inclusion removal from the steel by the slag layer. Monitoring the turbulent kinetic on the slag layer showed that the maximum turbulent kinetic did not increase from the optimum of case study 3. The optimum dam position was as close to the shroud as possible with the highest allowable height. Although this configuration is good for inclusion removal, it is very bad from a yield perspective unless draining holes are added. This showed the importance of the correct formulation of the optimisation problem. If a value like yield does not form part of the optimisation formulation, the optimiser ignores these values and undesirable optimum designs can be obtained.

## **4-6 CONCLUSION**

This chapter applied the methodology developed in Chapter 3 to different test cases. The first case optimised the position of a dam and a weir of a single-strand tundish. Two optimisation formulations were considered in this case, the first was the minimisation of the dead volume in the tundish and the second the maximisation of the inclusion removal of the tundish. Two different optima were obtained for the two different formulations, highlighting the importance of the correct formulation of the optimisation problem.

The second case optimised the baffle and pouring box area of a two-strand continuous caster. In this case, the minimum residence time was maximised by changing the geometry of the pouring box and baffle area. In this optimisation formulation a weighted value of the minimum residence time at the operating condition and that of the minimum residence time at a transition level were used. Significant improvements, in excess of 130%, were made to the design compared to the starting design.

The third case investigated the design of a new impact pad. An impact pad in a tundish has as its aim the reduction of turbulence in the tundish. For this reason the surface turbulent kinetic energy was minimised by changing the geometry of the impact pad.

The inclusion removal capabilities of the impact pad on its own, as optimised in the third test case, are not very good. The last case optimised a dam height and position in conjunction with the previously designed impact pad. The dam improved the particle removal capabilities of the tundish without increasing the turbulent kinetic energy on the free surface, but the suggested design seems to be impractical. This again highlights the importance of the correct formulation of the optimisation problem.

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## CHAPTER 5: CONCLUSION

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The continuous casting process is not a very old manufacturing process, but in the last four decades, it became the most common process for producing most basic metals. One of the particular important components in this system is the tundish. Traditionally, the tundish acted as a reservoir between the ladle and the mould but more recently it has been used as a grade separator, an inclusion removal device and a metallurgical reactor. A continuous drive to understand the molten metal flow patterns inside the tundish has led to many research papers being published in the modelling of the flow patterns, through either water modelling or numerical modelling. Included in these papers, researchers changed the design of the tundish by adding tundish furniture or changing the dimensions of the tundish. They showed that these changes can improve the flow patterns that ultimately improve the performance of the tundish. These changes were however based on trial-and-error experimentation or relied on the experience of the modeller to propose the design changes. This type of design methodology can lead to non-optimal solutions.

In this thesis, a methodology has been developed to optimise the molten steel flow patterns in a tundish by changing the tundish and tundish furniture. The methodology makes use of mathematical optimisation and Computational Fluid Dynamics (CFD) to give an optimum tundish and tundish furniture design based on certain design criteria as specified by the engineer. A literature survey that describes CFD modelling of a tundish and the optimisation algorithms used in this work were presented in Chapter 2.

The proposed methodology (as outlined in Chapter 3) consists of a number of steps. The first step is the validation of the numerical (CFD) model. This can be achieved by

either comparing the numerical results to a water model or to a plant trial. The second and most important step is the formulation of the optimisation problem. This step involves deciding on the design variables, objective function and constraint function(s). The last step before running the optimisation involves the automisation of the optimisation process. This involves the creation of appropriate files and scripts so that the CFD model can be created, solved and data extracted for a specific set of design variables without user intervention.

The methodology developed in the thesis was tested on four cases as described in Chapter 4. The first case optimised a simple dam-weir configuration for the lowest dead volume and for high inclusion removal on the slag layer. The second case optimised the baffle and pouring-box area in order to maximise the minimum residence time. In the third case, the methodology was used to design a new impact pad to reduce the slag layer turbulence. The newly designed impact pad was built and tested in the full-scale water model at the University of Pretoria. The new impact pad has also undergone trials in the single-strand continuous caster of Columbus Stainless Steel. The fourth and last case, described the optimisation of the position and height of a dam to be used with the impact pad developed in the third case, in order to increase the trapping of inclusion by the slag layer.

The methodology proved to work extremely well in all cases. The results show good improvements in the performance of the tundishes under investigation. From this, it is concluded that this methodology provides an improved alternative over the traditional design methods of developing and redesigning tundish and tundish furniture.

An important aspect that was highlighted by the study is that the correct formulation of the optimisation problem is crucial for the success of the optimisation procedure. This correct formulation is reliant on the understanding and skill of the design engineer. The resulting optimum is sensitive to the formulation of the optimisation problem.

One drawback of this methodology is the computational time that the optimisation procedure takes. This time can be reduced by using multiple computers to run the

simulations in parallel. The continued growth of computer power is leading to a reduction in the required optimisation time, but at the same time allowing more detailed CFD model to be constructed. This drawback is however offset by the fact that an optimum design is obtained which would not be possible or highly unlikely using traditional experimental modelling (water modelling or plant trials) or trial-and-error numerical modelling.

The methodology developed can now be applied in general to other tundishes with other tundish furniture, providing that the design engineer formulates the optimisation problem correctly.

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## CHAPTER 6: RECOMMENDATIONS AND FUTURE WORK

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A number of new areas that can follow on this current research have been identified and are given below.

### **6-1 APPLICATION OF METHODOLOGY TO OTHER ELEMENTS OF THE CONTINUOUS CASTING PROCESS**

The optimisation methodology developed in this study should be applied to the Submerged Entry Nozzle (SEN), mould design and other components downstream of the tundish in the continuous casting process. It is important to have favourable flow patterns in the mould as poor flow patterns can result in slag entrainment that will render all the improvements made in the tundish useless. If electromagnetic stirring is used in the mould, the operating parameters of the stirrer could be optimised.

The optimisation methodology should also be applied to components upstream of the tundish, e.g., the ladle. This could include the optimum design of gas sparging in the ladle to reduce temperature stratification, or the design of the refractory to minimise the heat losses from the ladle.

### **6-2 TRANSIENT COMPUTATIONAL FLUID DYNAMICS MODEL**

The cases in the thesis were all steady state. As the actual tundish and ladle operation involves transient periods as well, especially during mixed grade transition, the optimisation of the transient performance can also be treated with this methodology as computing power allows.



The cascading that corresponds to high oxidation of the steel also occurs during the initial filling (first heat) of the tundish. This transient filling phenomenon and design of the furniture to reduce this effect can also be treated with this methodology.

### **6-3 TESTING OF OPTIMISATION FORMULATIONS**

Additional tundish and tundish furniture designs can be optimised and the methodology can be tested on some of the other optimisation formulations given in Chapter 3. Some of the optimisation formulations at the time of this study were computationally too expensive, but with the rapid growth in computational power, these formulations could soon be investigated.

### **6-4 EXTENSION AND VALIDATION OF INCLUSION MODELLING**

Validation of the inclusion modelling should be undertaken to validate the accuracy of the models when using stochastic tracking. There remains some uncertainty as to the accuracy of the CFD model of the small inclusions in a turbulent flow field.

A model should also be developed to include the detailed chemistry of the inclusions in the CFD analysis. This model should include aspects such as inclusion generation, amalgamation, and reaction with the slag layer. In this study, a particle touching the free surface was assumed to be trapped which is not the case in a physical tundish. A first attempt was made to improve the modelling of the capturing of a particle on the slag surface. For this purpose, a FLUENT User Defined Function was developed and is given in Appendix H. This first attempt is a simple model and calculates the maximum continuous time that a particle spends in a user-defined region close to the slag layer. A correlation is then used that relates the probability of a particle being trapped, to the size of the particle and the time it spent near the slag layer. Other possible correlations should also be investigated and the detailed reaction of the particle on the slag surface can be included. One of the anticipated difficulties for this future work is to get quantitative data from the plant operations to validate the numerical model.

The erosion of the tundish furniture is a further source of inclusions. A model describing the erosion rate of the furniture and the corresponding size and chemical composition of the inclusions that are introduced into the steel should be developed. The movement of these inclusions and interaction with the slag layer should then be modelled in a similar manner as described in the paragraph above.

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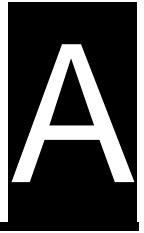
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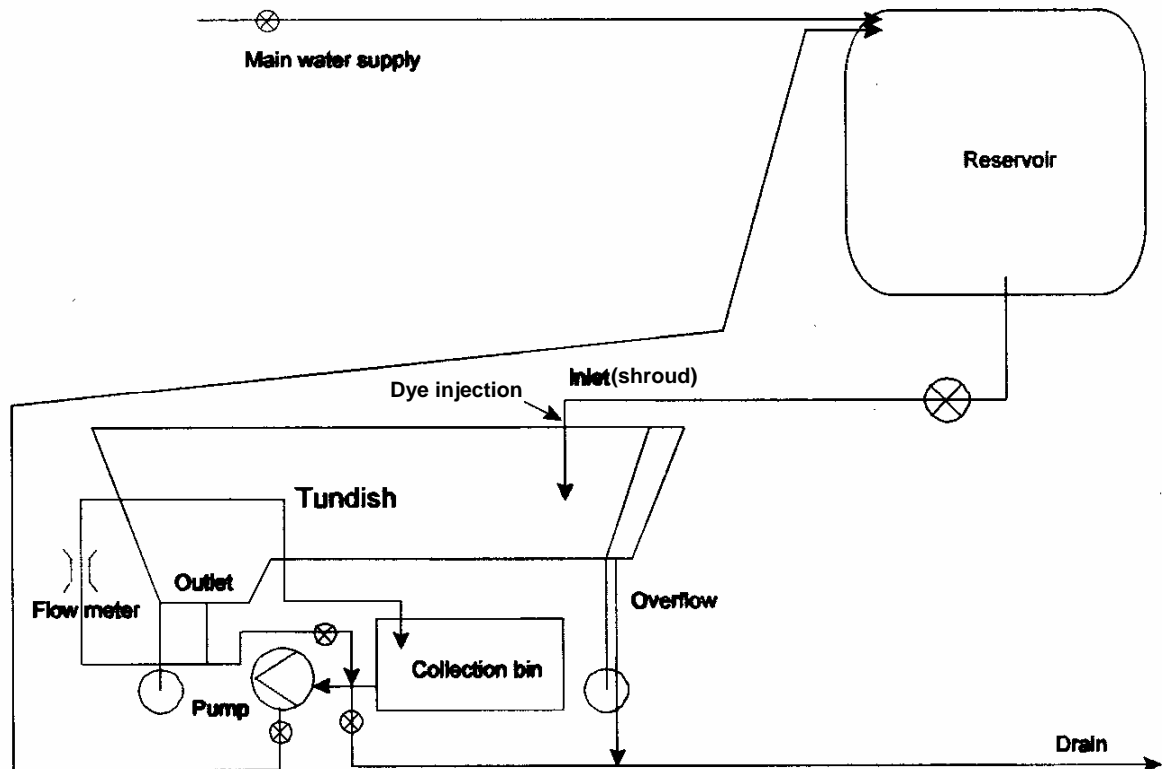
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## APPENDIX A: WATER MODEL VALIDATION STUDY

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### A-1 INTRODUCTION

An important part of the optimisation is to trust the accuracy of the numerical model. For this purpose a water model validation study was done. This work was published in Mechanical Technology [65]. The details of this study are given in this appendix. In physical modelling, water is normally used to simulate molten steel in perspex models of tundishes. In this modelling, emphasis has been placed on the matching of Reynolds (Re) and Froude (Fr) similarity criteria [17]. When water at room temperature is used as the modelling fluid, matching of both Reynolds and Froude numbers require the use of full-scale models. In reduced-scale models, either Reynolds or Froude numbers can be satisfied. A full-scale water model of the Columbus Stainless Steel tundish was commissioned at the University of Pretoria in 1999 [66] therefore having the advantage of having both Reynolds and Froude number similarity satisfied. The tundish model is constructed from 10mm-thick perspex sheets and supported by a steel frame. The water flow network provides the option to recirculate the water from the tundish outlet to the reservoir, or to divert it to a drain (see Figure A-1).



**Figure A-1: Schematic layout of the water model**

In water modelling studies, a pulse of tracer such as dye or a salt solution is injected in the incoming water stream while its concentration at the outlet is measured as a function of time. The plot of the exit concentration against time is known as the residence time distribution (RTD) curve. The RTD of a fluid in the tundish is used to characterise the fluid flow. The RTD is commonly used to determine the volumes of plug flow, mixed flow and dead regions in the tundish. The use of dye as tracer also facilitates the visual observation of the flow patterns through the tundish and helps in identifying the locations of slow moving or turbulent and well-mixed regions.

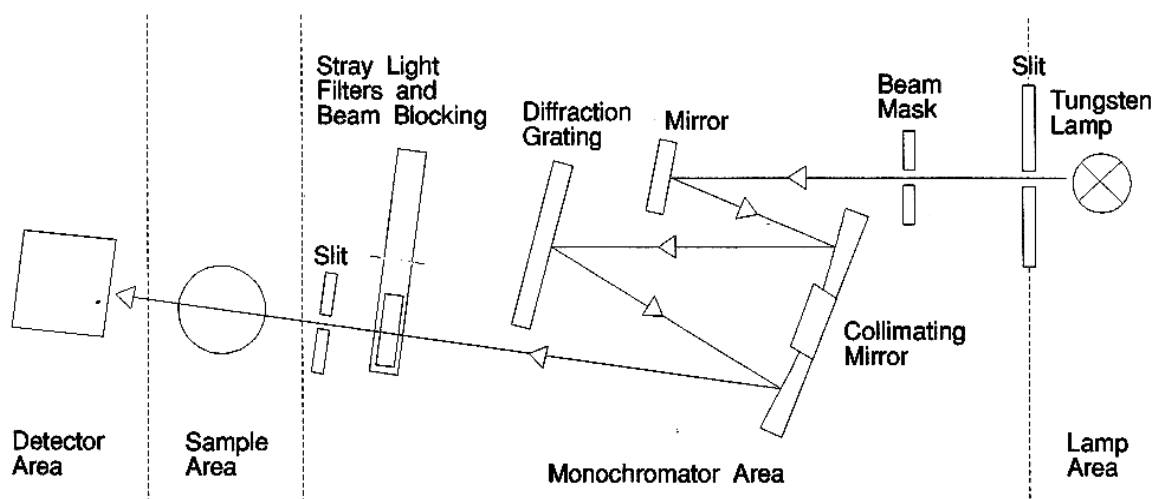
In mathematical modelling, the turbulent Navier-Stokes equations are solved with appropriate boundary conditions to yield detailed information on velocity, pressure and turbulence fields in the tundish. Such models can also be used to theoretically determine the residence time distribution of fluid in the tundish by releasing a passive scalar at the inlet and tracking its concentration distribution through time at the outlet.

## **A-2 EXPERIMENTAL SETUP**

The experimental process involves achieving a stable operating level in the tundish for a period which is at least 3 times the average residence time before an experiment is initiated by injecting the dye. A water sample is obtained from a sampling tube inside the outlet pipe. The water sample is fed through a spectrophotometer where the absorbance at a specified wavelength is measured. The absorbance of the sample is referenced to the absorbance of clean water. A pre-measured amount of the dye solution is injected into the shroud (inlet to the tundish) as a pulse over three to five seconds. The dye input is called the tracer and the mixing of the tracer in the water changes the absorbance of the water.

### **A-2.1 SPECTROPHOTOMETER**

A Novaspec II visible spectrophotometer [67] was used to determine the residence time distribution curve of the tracer at the outlet of the water model. The spectrophotometer provides measurement of both light absorbance and light transmission in the visible wavelength range (325–900nm). The diagram in Figure A-2 shows in simplified form the optical system of the instrument. The light output from the lamp passes through a slit into the monochromator where a collimating mirror converts the light into a parallel beam. The light then passes to the diffraction grating to produce light of the selected wavelength. This monochromatic light then passes through the stray light filters and the monochromator outlet slit and then through the cuvette with the water sample to the solid-state detector unit.



**Figure A-2: The spectrophotometer's optical system [67]**

The relationship between the concentration of the sample and its absorbance is linear, and hence absorbance is widely used experimentally. The absorbance ( $A$ ) is calculated from the logarithm of the sample transmittance ( $T$ ) by applying the Beer-Lambert law  $A = \log 100/T$ . The result is displayed in units of absorbance. In order to calculate the transmittance, the instrument measures the amount of light at the specified wavelength that has passed through the sample and compares it with that which has passed through the reference. The dye used in the experiment has a wavelength of 435nm.

### **A-2.2 DIGITAL CAMCORDER**

A Sony TRV110 digital camcorder is used to capture the experiment digitally on video. This digital video is then transmitted via an IEEE 1394 Firewire interface to a PC for further digital editing and processing.

### **A-2.3 ULTRASONIC FLOW METER**

The Altosonic Ultrasonic Flow Meter [66] is a portable flow meter that can be readily attached to existing pipelines. Measurement is performed without any obstruction to the flow of the medium and no alterations to the pipe section involved are necessary, thus no additional pressure loss will occur. A sound wave that is sent in the direction of the flow through a medium will travel faster

than one that is sent in the opposite direction. This principle is used in the ultrasonic transit time flow meter.

## A-3 RESULTS

### A-3.1 RESIDENCE TIME DISTRIBUTION (RTD)

The RTD curve of the experiment (repeated four times) is compared to the RTD curves obtained by the CFD code in Figure A-3 for an empty tundish. Different turbulence modelling options were tested in the CFD model and the one shown (RNG k- $\epsilon$  turbulence model) gave the best results. The experimental set-up was emulated by a 2 sec pulse injection in the CFD model to obtain the RTD.

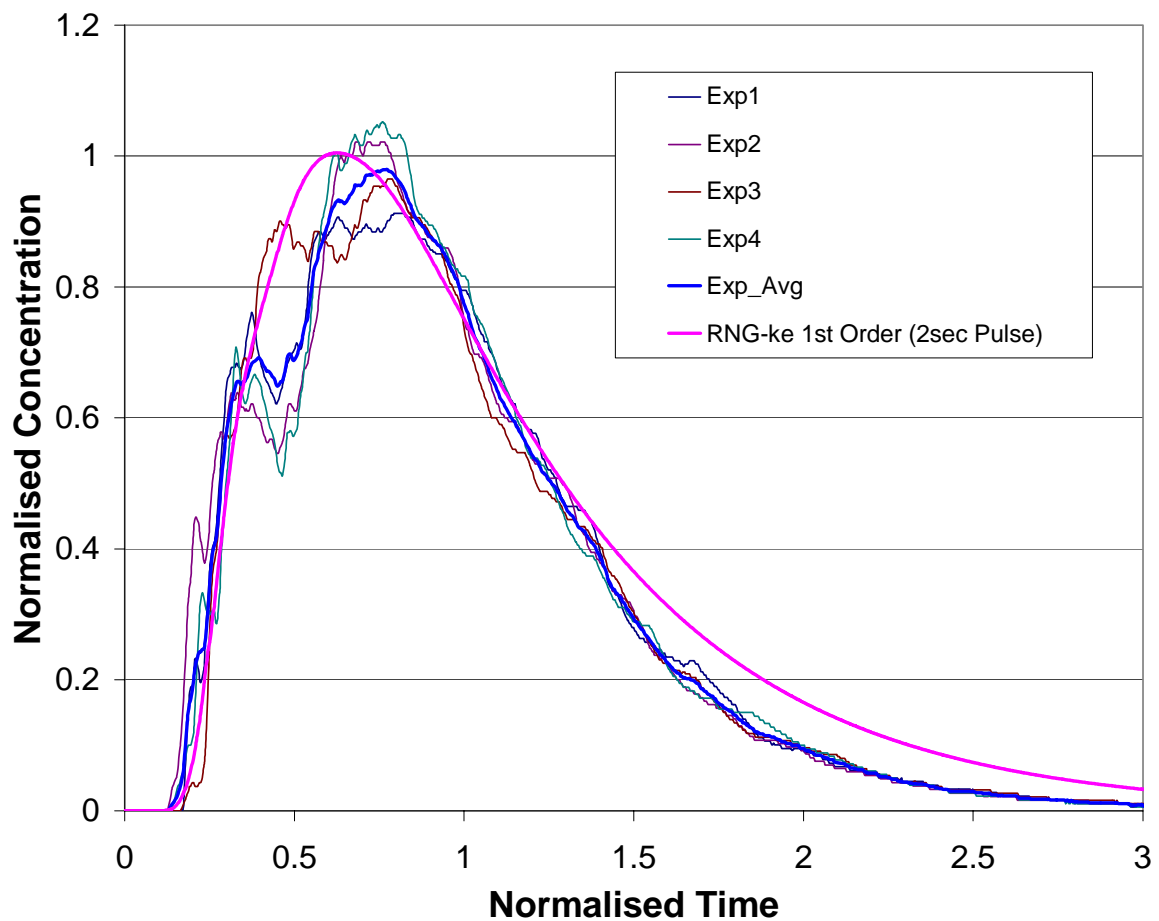


Figure A-3: Comparison of RTD curves

From the RTD curve the relevant RTD data were extracted to compare the experimental and CFD data. These data are given in Table A-1. Generally, good agreement is found between the experimental and CFD data with the Minimum Residence Time (MRT) being the only value that is not predicted to within 15%. This MRT is however very sensitive to the time that the injection took and the sensitivity of the spectrophotometer.

**Table A-1: Comparison of RTD data of the water model and CFD model**

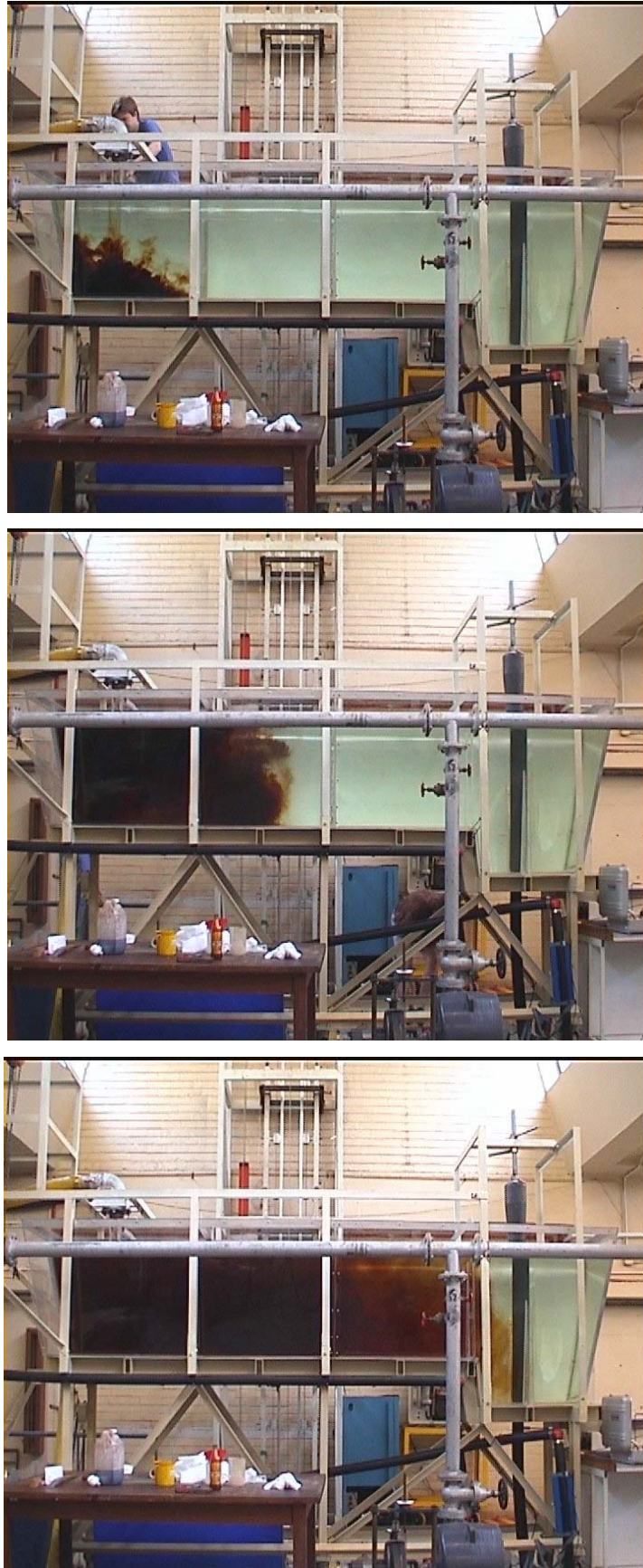
	Water model	CFD	% Difference
MRT	0.128	0.154	20.3%
Dispersed Plug Flow ( $V_{dpv}$ )	0.450	0.391	13.1%
Mixed Flow ( $V_{mv}$ )	0.406	0.452	11.3%
Dead Volume ( $V_{dv}$ )	0.144	0.156	8.3%

### **A-3.2 COMPARISON OF FLOW PATTERNS**

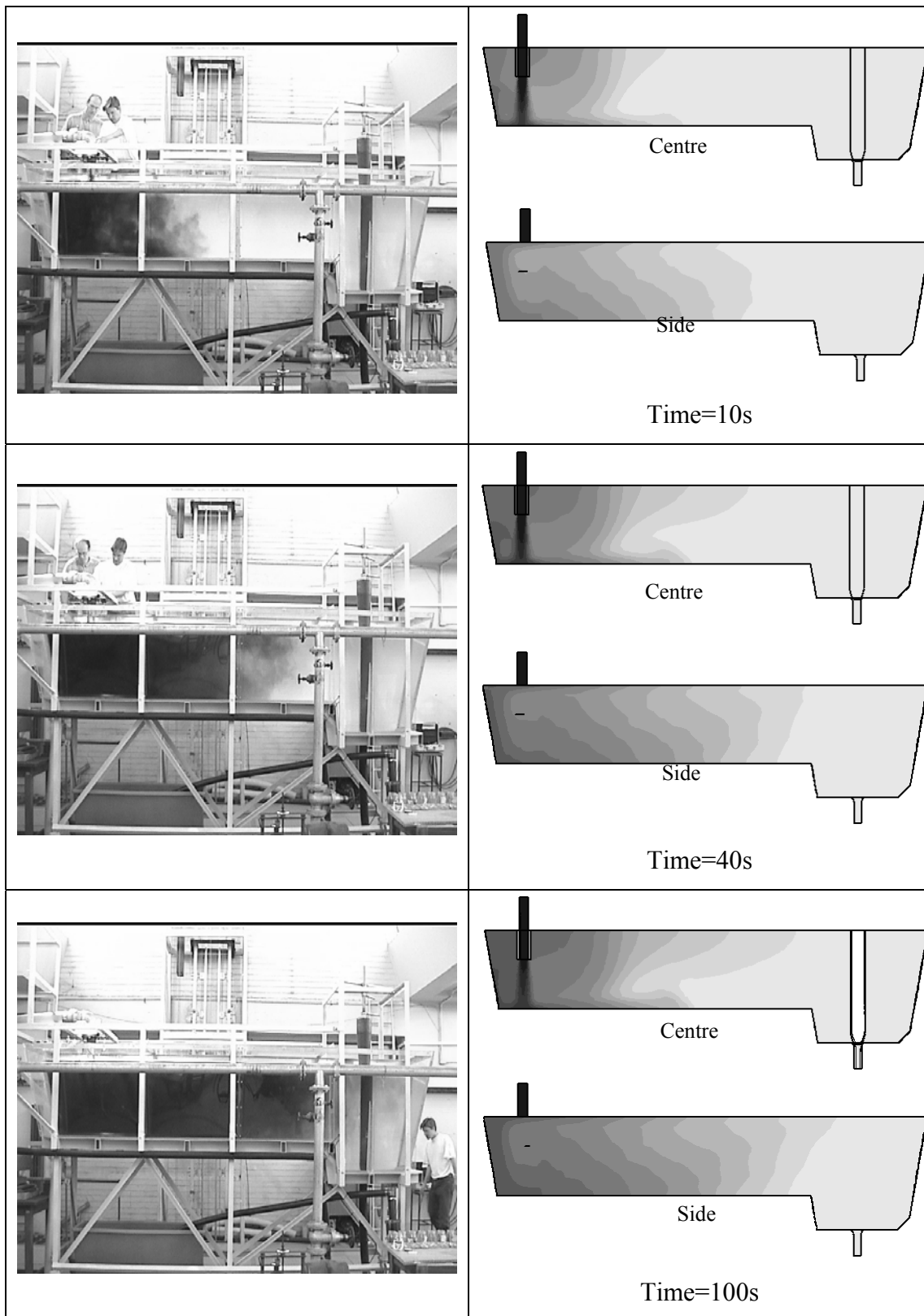
Three frames captured by the digital video and given in Figure A-4 show the dye pattern at different times after the dye has been injected. The first frame shows the dye pattern just after the injection of the dye. In the second frame the dye started to move towards the outlet in a uniform pattern. In the last frame the short circuiting to the outlet can be clearly seen.

A comparison between the experimental and numerical results is given in Figure A-5. The numerical results show the scalar concentration on the centre line and side of the tundish. In general the patterns are similar for the experimental and numerical results. The numerical results show that there is significant variation between the centre and side of the tundish.





**Figure A-4: Dye flow patterns at different times after dye injection**



**Figure A-5: Comparison between the experimental (left) and numerical (right) results. The numerical results show the scalar concentration.**

#### **A-4 CONCLUSION AND FUTURE WORK**

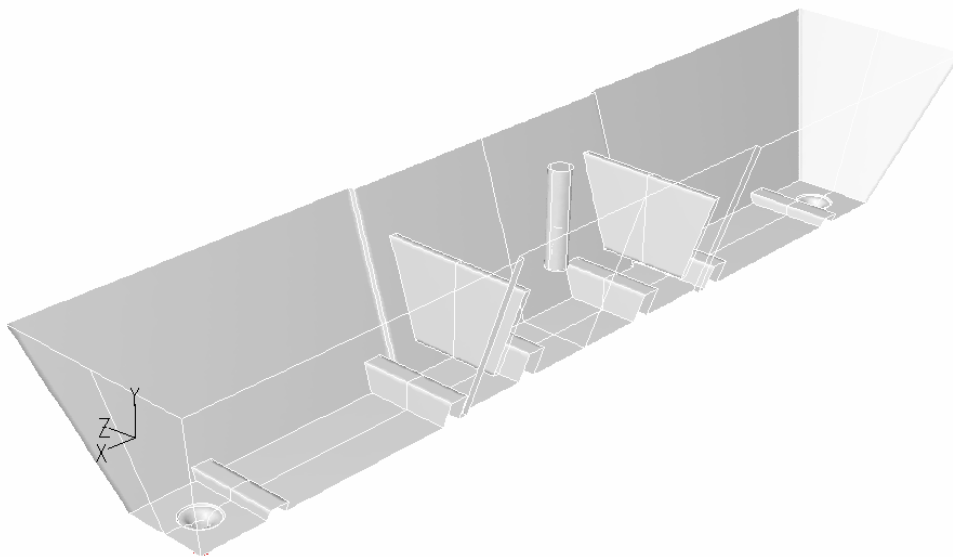
There appears to be a good correlation between the experimental results and the CFD results for this simple set-up. The diffusion of the tracer during the experiment could also not be quantified.

---

## APPENDIX B: PLANT TRIAL VALIDATION STUDY

---

A validation study between experimental plant data and the CFD modelling was carried out to ensure that the CFD modelling techniques used are calibrated. The validation was done on the V1-V2 continuous caster of ISCOR Vanderbijlpark, South Africa. The configuration used for the trial is shown in Figure B-1.



**Figure B-1: Tundish configurations for validation study**

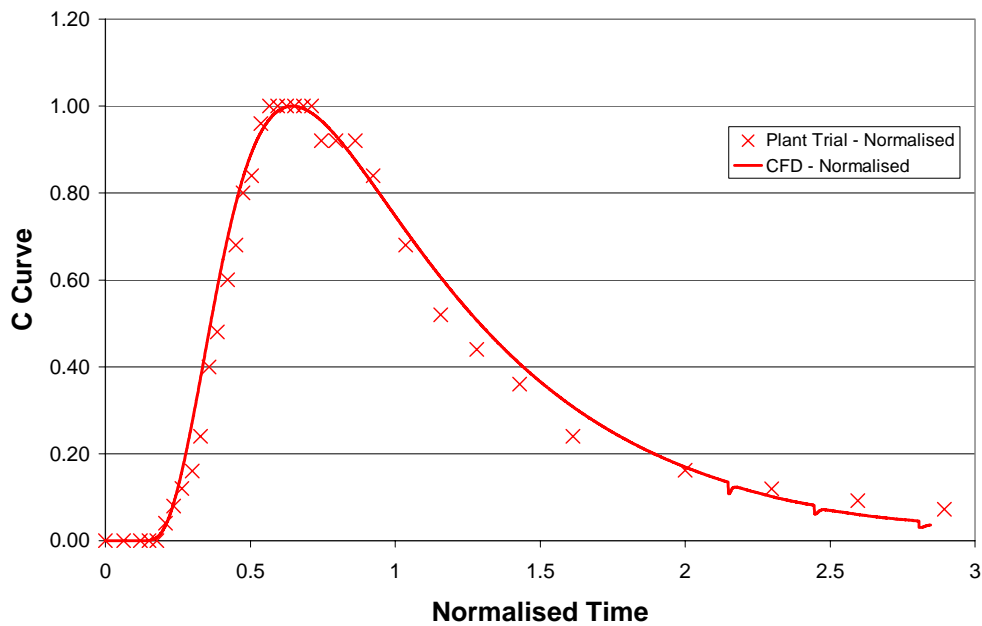
Table B-1 gives the details of the CFD model used in the validation study.

**Table B-1: Details of CFD model used in validation study**

<b>Description</b>	<b>Setting</b>
Model	Non-isothermal steady state flow, turbulence and heat transfer, transient species concentration
Turbulence model	Standard $k-\epsilon$
Discretisation scheme	2 <sup>nd</sup> order for pressure 2 <sup>nd</sup> order upwind for all other equations
Liquid Steel property:	
Reference density	7026.8kg/m <sup>3</sup>
Reference temperature	1800K
Thermal conductivity	52.5W/m·K
Viscosity	0.0053kg/m·s
Thermal expansion coefficient	$1.197 \times 10^{-4} \text{K}^{-1}$
Inlet boundary condition:	
Mass flow	16.67kg/s (quarter model)
Inlet temperature	1856.15K
Inlet turbulence intensity	10%
Inlet hydraulic diameter	0.1025m
Outlet boundary condition:	Zero gradient for all equations normal to boundary
Wall boundary condition:	
Bottom effective heat transfer coefficient	1.25W/m <sup>2</sup> ·K
Side effective heat transfer coefficient	2.76W/m <sup>2</sup> ·K
Slag effective heat transfer coefficient	11.4W/m <sup>2</sup> ·K
Free stream temperature	298.15K
Remaining walls (dam, baffles, etc.)	Adiabatic

A copper trace experiment was conducted on-site, which involved the introduction of copper next to the shroud and then periodically taking samples from the mould. The copper concentration in the samples was measured using a photo-spectrometer [28, 29]. A comparison of the CFD-predicted RTD curve and the measured points is shown in Figure B-2. It can be seen in this figure that the plant trial and CFD are in good agreement. The RTD data extracted from these curves are given in Table B-2.

It is mainly the dead flow volume that differs significantly with the plant trial results. The comparison is however fairly good taking into account all the uncertainties associated with the plant trial. For example, the path of the tracer differs between the plant trial and numerical model, as the copper is introduced into the tundish next to the shroud on-site and in the CFD model the tracer is introduced in the shroud.



**Figure B-2: Comparison of RTD curves of the plant trial and CFD model**

**Table B-2: : Comparison of RTD data of the plant trial and CFD model**

	Plant Trial	CFD	% Error
Plug flow volume [%]	20.7	18.2	11.9
Mixed flow volume [%]	74.5	75.7	1.6
Dead flow volume [%]	4.8	6.1	27.1



## APPENDIX C: MODIFIED DYNAMIC-Q PROGRAM

The Dynamic-Q program was modified to be able to link to Fluent and Gambit. The complete program listing in Fortran is given in this appendix. The modification made to the programme is the automatic linking with Fluent and Gambit as well as the automatic extraction of the data (refer to system call in especially fch77.for).

### driver77.for

```

PROGRAM DRIVER77
C*****C
C
C      DYNAMIC-Q ALGORITHM FOR CONSTRAINED OPTIMIZATION      C
C
C      Sample driver for the subroutine DynQ77                  C
C
C
C
C!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!C
C
C  User specified subroutines:                                  C
C
C  The objective function and constraint functions must be specified C
C  in subroutine FCH. Expressions for the respective gradient vectors C
C  must be specified in subroutine GradFCH.                    C
C
C  {The user may compute gradients by finite differences if necessary C
C   - see example code in GradFCH}                             C
C
C  Side constraints should not be included as inequality constraints C
C  in the above subroutines, but entered in the relevant section below.C
C
C  Further quantities to be specified are the number of variables N, C
C  starting point X, number of inequality NP, equality NQ, lower NL C
C  and upper limits NU. Also specify the move limit DML and C
C  convergence tolerances on step size and function value XTOL and C
C  FTOL and maximum number of iterations KLOOPMAX.           C
C
C!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!C
C
C  The application of the code is illustrated here for the very simple C
C  but general example problem (Hock 71):                      C
C
C      minimize  F(X) = X(1)*X(4)*(X(1)+X(2)+X(3))+X(3)        C
C  such that
C
C              C(X) = 25-X(1)*X(2)*X(3)*X(4) <= 0           C
C
C      and
C
C              H(X) = X(1)**2+X(2)**2+X(3)**2+X(4)**2-40 = 0   C
C
C      and side constraints
C
C              1 <= X(I) <= 5 , I=1,2,3,4                    C
C
C  The remainder of the code is self-explanatory. Read the comments C

```

## Appendix C: Modified Dynamic-Q Program

```

C below for the specification of initial data and parameter settings. C
C                                                                 C
C*****C
C
      IMPLICIT REAL*8 (A-H,O-Z),INTEGER(I-N)
      PARAMETER (NMAX=300,NLMAX=50,NUMAX=50)
      LOGICAL PRNCONST,FEASIBLE
      DIMENSION X(NMAX)
      DIMENSION NLV(NLMAX),NUV(NUMAX),V_LOWER(NLMAX),V_UPPER(NUMAX)
      DIMENSION DELTX(NMAX),DML(NMAX)
C
C*****OPEN OUPUT FILES*****C
C
      OPEN (9,FILE='Lfopc.out')
      OPEN (10,FILE='Approx.out')
      OPEN (11,FILE='DynamicQ.out')
C
C*****SPECIFY NUMBER OF VARIABLES N *****C
C                                                                 C
      N=6
C
C*****SPECIFY STARTING POINT (INITIAL GUESS) : X(I), I=1,N *****C
C                                                                 C
      PI=4.D0*DATAN(1.0D0)
C
      DO I=1,N
      X(I)=8.D-1
      END DO

      X(1)=650.
      X(2)=400.
      X(3)=50.
      X(4)=50.
      X(5)=20.
      X(6)=20.
C
C*****SPECIFY NUMBER OF INEQUALITIES NP (NP=0 IF NONE)*****C
C (EXCLUDING SIDE CONSTRAINTS WHICH SHOULD BE SEPARATELY C
C SPECIFIED BELOW) C
C                                                                 C
      NP=1
C
C*****SPECIFY NUMBER OF EQUALITIES NQ (NQ=0 IF NONE)*****C
C                                                                 C
      NQ=0
C
C*****SPECIFY SIDE CONSTRAINTS*****C
C
      Indicate the number of lower limits NL and upper limits NU
      (0<=NU<=N and 0<=NL<=N)
      NL=N
      NU=N
C
      Specify LOWER limits with V_LOWER(j) specifying the VALUE of
      the limit and NLV(j)=I the associated VARIABLE X(I), j=1,NL
      IF (NL.GT.0) THEN
      DO I=1,NL
          NLV(I)=I
      END DO

      DO I=1,NL
          V_LOWER(I)=-90.0
      END DO

      V_LOWER(1)=400.
      V_LOWER(2)=300.

```



*Appendix C: Modified Dynamic-Q Program*

```

V_LOWER(3)=40.
V_LOWER(4)=0.
V_LOWER(5)=0.
V_LOWER(6)=0.

END IF

C Specify UPPER limits with V_UPPER(j) specifying the VALUE of
C the limit and NUV(j)=I the associated VARIABLE X(I), j=1,NU
IF (NU.GT.0) THEN

DO I=1,NU
    NUV(I)=I
END DO

c DO I=1,NU
c     V_UPPER(I)=0.0
c END DO

V_UPPER(1)=1200.
V_UPPER(2)=600.
V_UPPER(3)=10000.
V_UPPER(4)=100.
V_UPPER(5)=100.
V_UPPER(6)=40.

END IF

C
C*****GIVE THE CONVERGENCE TOLERANCES ON FUNC AND STEP NORM VALUES*****C
C
    FTOL=1.D-8

    XTOL=1.D-5

C
C*****SPECIFY THE MOVE LIMIT DML*****C
C
c DO I=1,N
c     DML(I)=30.0
c END DO

DML(1)=200.
DML(2)=100.
DML(3)=10.
DML(4)=25.
DML(5)=25.
DML(6)=10.

C
C*****GIVE THE MAXIMUM NUMBER OF ITERATIONS*****C
C
    KLOOPMAX=99

C
C*****PRINT CONSTRAINTS TO SCREEN AT END OF PROGRAM?*****C
C
    YES: .TRUE.      OR      NO: .FALSE.
C
    PRNCONST=.TRUE.

C
C*****SPECIFY SIZE OF FINITE DIFFERENCE STEP SIZE*****C
C
c DO I=1,N
c     DELTX(I)=10.0
c END DO

DELTX(1)=100.
DELTX(2)=50.
DELTX(3)=5.
DELTX(4)=12.
DELTX(5)=12.

```

## Appendix C: Modified Dynamic-Q Program

```

DELT(6)=5.

C
C*****FEASIBLE LIMIT TO CHECK CONVERGENCE*****C
C      (AMOUNT AN CONSTRAINT CAN BE VIOLATED)
C
C      FEASLIM=1.D-1
C
C
C*****CALL SUBROUTINE DYNQ77*****C
C      CALL DYNQ77(N,X,NP,NQ,NL,NU,NLV,NUV,V_LOWER,V_UPPER,
C      *          FTOL,XTOL,DML,KLOOPMAX,PRNCONST,DELT,FEASLIM)
C
C      STOP
C      END PROGRAM DRIVER77

```

## DynQ77.for

```

SUBROUTINE DYNQ77(N,X,NP,NQ,NL,NU,NLV,NUV,V_LOWER,V_UPPER,
*          FTOL,XTOL,DML,KLOOPMAX,PRNCONST,DELT,FEASLIM)
C*****C
C      DYNAMIC-Q ALGORITHM FOR CONSTRAINED OPTIMIZATION
C      GENERAL MATHEMATICAL PROGRAMMING CODE (FORTRAN 77)
C      -----
C
C      Programmed by A.M. HAY
C      Multidisciplinary Design Optimization Group (MDOG)
C      Department of Mechanical Engineering, University of Pretoria
C      June 2000
C
C      UPDATED : 18 August 2000
C
C      Specific modification made to code for implementation into
C      Fluent by DJ de Kock 2003
C
C      This code is based on the Dynamic-Q method of Snyman documented
C      in the paper "THE DYNAMIC-Q OPTIMIZATION METHOD: AN ALTERNATIVE
C      TO SQP?" by J.A. Snyman and A.M. Hay. Technical Report, Dept Mech.
C      Eng., UP.
C
C      BRIEF DESCRIPTION
C      -----
C
C      Dynamic-Q solves inequality and equality constrained optimization
C      problems of the form:
C
C      minimize F(X) , X={X(1),X(2),...,X(N)}
C      such that
C      Cj(X) <= 0          j=1,2,...,NP
C      and
C      Hj(X) = 0          j=1,2,...,NQ
C      with lower bounds
C      CLj(X) = V_LOWER(j)-X(NLV(j)) <= 0   j=1,2,...,NL
C      and upper bounds
C      CUj(X) = X(NUV(j))-V_UPPER(j) <= 0   j=1,2,...,NU
C
C      This is a completely general code - the objective function and the
C      constraints may be linear or non-linear. The code therefore solves
C      LP, QP and NLP problems.
C
C      C!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!C
C
C      Arguments of DynQ77 subroutine:

```

## Appendix C: Modified Dynamic-Q Program

```

C
C NAME      DIMENSION  TYPE      DESCRIPTION
C N          X(N)      INTEGER   Number of variables
C X          X(N)      DBL PREC  Starting point
C NP         X(N)      INTEGER   Number of inequality constraints
C NQ         X(N)      INTEGER   Number of equality constraints
C NL         X(N)      INTEGER   Number of lower bounds
C NU         X(N)      INTEGER   Number of upper bounds
C NLV        NLV(NL)   INTEGER   See description below
C NUV        NUV(NU)   INTEGER   See description below
C V_LOWER    V_LOWER(NL) DBL PREC  See description below
C V_UPPER    V_UPPER(NL) DBL PREC  See description below
C FTOL              DBL PREC  Termination tolerance on func. value
C XTOL              DBL PREC  Termination tolerance on step size
C DML              DBL PREC  Move limit
C KLOOPMAX        INTEGER   Maximum number of iterations
C PRNCONST        LOGICAL   Controls printing of constraints to
C                  screen at end of program
C DELTX          DELTX(N)   DBL PREC  Size of finite difference
C DML            DML(N)     DBL PREC  Move limit for each variable
C FEASLIM                DBL PREC  Amount a constraint can be violated
C
C!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!C
C
C      Specify LOWER limits with V_LOWER(j) specifying the VALUE of
C      the limit and NLV(j)=I the associated VARIABLE X(I), j=1,NL
C      Specify UPPER limits with V_UPPER(j) specifying the VALUE of
C      the limit and NUV(j)=I the associated VARIABLE X(I), j=1,NU
C
C!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!C
C
C The application of the code is illustrated here for the very simple
C but general example problem (Hock 71):
C
C      minimize F(X) = X(1)*X(4)*(X(1)+X(2)+X(3))+X(3)
C such that
C              C(X) = 25-X(1)*X(2)*X(3)*X(4) <= 0
C      and
C              H(X) = X(1)**2+X(2)**2+X(3)**2+X(4)**2-40 = 0
C
C      and side constraints
C
C              1 <= X(I) <= 5 , I=1,2,3,4
C
C
C The remainder of the code is self-explanatory. Read the comments
C below for the specification of initial data and parameter settings.
C
C*****C
C
C      IMPLICIT REAL*8 (A-H,O-Z),INTEGER(I-N)
C      DIMENSION X(N),DELX(N),GF(N),GC_V(N),GH_V(N)
C      DIMENSION C(NP),GC(NP,N),BCURV(NP)
C      DIMENSION H(NQ),H_A(NQ),GH(NQ,N),CCURV(NQ)
C      DIMENSION NLV(NL),NUV(NU),V_LOWER(NL),V_UPPER(NU)
C      DIMENSION C_A(NP+NL+NU+N)
C      DIMENSION X_H(0:KLOOPMAX,N),F_H(0:KLOOPMAX)
C      DIMENSION C_H(0:KLOOPMAX,NP+NL+NU+N),H_H(0:KLOOPMAX,NQ)
C      LOGICAL PRNCONST,FEASIBLE
C      DIMENSION DELTX(N),DML(N)
C
C
C#####C
C*****C
C      MAIN PROGRAM FOLLOWS:
C*****C
C#####C
C

```

## Appendix C: Modified Dynamic-Q Program

```

C*****INITIALIZE OUTPUT*****C

WRITE (10, '(1X, "DYNAMICQ OUTPUT FILE")')
WRITE (10, '(1X, "-----")')
WRITE (10, '(1X, "Number of variables [N]=", I3)', N
WRITE (10, '(1X, "Number of inequality constraints [NP]=", I3)', NP
WRITE (10, '(1X, "Number of equality constraints [NQ]=", I3)', NQ
WRITE (10, '(1X, "Move limit=", 5F12.8)', (DML(I), I=1, N)
WRITE (*, '(1X, "DYNAMICQ OPTIMIZATION ALGORITHM")')
WRITE (*, '(1X, "-----")')
WRITE (*, '(1X, A)') 'Iter Function value ? XNORM RFD'
WRITE (*, '(1X, A)') '-----'
WRITE (11, '(1X, "DYNAMICQ OPTIMIZATION ALGORITHM")')
WRITE (11, '(1X, "-----")')
WRITE (11, '(1X, A)')
* 'Iter Function value ? XNORM RFD'
WRITE (11, '(5(1X, A, I2, A, 8X))') ('X(', I, ')', I=1, N)

C Initialize outer loop counter
KLOOP=0

C Arbitrary large values to prevent premature termination
F_LOW=1.D6
RFD=1.D6
RELXNORM=1.D6

DO I=1, (NP+NL+NU+N)
  C_A(I)=0.D0
END DO

C Specify initial approximation curvatures
ACURV=0.D0
DO I=1, NP
  BCURV(I)=0.d0
END DO
DO I=1, NQ
  CCURV(I)=0.D0
END DO

C*****START OF OUTER OPTIMIZATION LOOP*****C

DO WHILE (KLOOP.LE.KLOOPMAX)

C*****APPROXIMATE FUNCTIONS*****C

C Determine function values
CALL FCH(N, NP, NQ, X, F, C, H, KLOOP, 0)

C Calculate relative step size
IF (KLOOP.GT.0) THEN
  DELXNORM=0.D0
  XNORM=0.D0
  DO I=1, N
    DELXNORM=DELXNORM+(X_H(KLOOP-1, I)-X(I))**2
    XNORM=XNORM+X(I)**2
  END DO
  DELXNORM=DSQRT(DELXNORM)
  XNORM=DSQRT(XNORM)
  RELXNORM=DELXNORM/(1.D0+XNORM)
END IF

C Determine lowest feasible function value so far
C FEASLIM=1.D-6
IF (KLOOP.GT.0) THEN
  FEASIBLE=.TRUE.
  DO I=1, NP
    IF (C(I).GT.FEASLIM) THEN
      FEASIBLE=.FALSE.
    
```

## Appendix C: Modified Dynamic-Q Program

```

        END IF
      END DO
      DO I=1,NQ
        IF (DABS(H(I)).GT.FEASLIM) THEN
          FEASIBLE=.FALSE.
        END IF
      END DO
      DO I=1,NL
        IF (C_A(I+NP).GT.FEASLIM) THEN
          FEASIBLE=.FALSE.
        END IF
      END DO
      DO I=1,NU
        IF (C_A(I+NP+NL).GT.FEASLIM) THEN
          FEASIBLE=.FALSE.
        END IF
      END DO
    END IF
  END IF

C   Calculate relative function difference
      IF (F_LOW.NE.1.D6.AND.FEASIBLE) THEN
        RFD=DABS(F-F_LOW)/(1+DABS(F))
      END IF

      IF (FEASIBLE.AND.F.LT.F_LOW) THEN
        F_LOW=F
      END IF

C   Store function values
      DO I=1,N
        X_H(KLOOP,I)=X(I)
      END DO
      F_H(KLOOP)=F
      DO I=1,NP
        C_H(KLOOP,I)=C(I)
      END DO
      DO I=1,NL
        C_H(KLOOP,NP+I)=C_A(NP+I)
      END DO
      DO I=1,NU
        C_H(KLOOP,NP+NL+I)=C_A(NP+NL+I)
      END DO
      DO I=1,N
        C_H(KLOOP,NP+NL+NU+I)=C_A(NP+NL+NU+I)
      END DO
      !   C_H(KLOOP,NP+NL+NU+1)=C_A(NP+NL+NU+1)
      DO I=1,NQ
        H_H(KLOOP,I)=H(I)
      END DO

C   Determine gradients
      CALL GRADFCH(N,X,NP,NQ,GF,GC,GH,F,C,H,DELTX,KLOOP)

C   Calculate curvatures
      IF (KLOOP.GE.1) THEN
        DELXNORM=0.D0
        DO I=1,N
          DELX(I)=X_H(KLOOP-1,I)-X_H(KLOOP,I)
          DELXNORM=DELXNORM+DELX(I)**2
        END DO
      END IF

C   Dot product of GF and DELX
      DP=0.D0
      DO I=1,N
        DP=DP+GF(I)*DELX(I)
      END DO

```

## Appendix C: Modified Dynamic-Q Program

```

          ACURV=2.*(F_H(KLOOP-1)-F_H(KLOOP)-DP)
*          /DELXNORM

          DO J=1,NP
C      Extract relevant vector from GC
          DO I=1,N
              GC_V(I)=GC(J,I)
          END DO

C      Dot product of GC_V and DELX
          DP=0.D0
          DO I=1,N
              DP=DP+GC_V(I)*DELX(I)
          END DO

C      Calculate corresponding curvature BCURV(J)
          BCURV(J)=2.*(C_H(KLOOP-1,J)-C_H(KLOOP,J)
*          -DP)/DELXNORM
          END DO

          DO J=1,NQ
C      Extract relevant vector from GC
          DO I=1,N
              GH_V(I)=GH(J,I)
          END DO

C      Dot product of GH_V and DELX
          DP=0.D0
          DO I=1,N
              DP=DP+GH_V(I)*DELX(I)
          END DO

C      Calculate corresponding curvature CCURV(J)
          CCURV(J)=2.*(H_H(KLOOP-1,J)-H_H(KLOOP,J)
*          -DP)/DELXNORM
          END DO
      END IF

C*****RECORD PARAMETERS FOR THE ITERATION*****C

C      Write approximation constants to Approx.out
      WRITE (10,'(/1X,A,I3)') 'Iteration ',KLOOP
      WRITE (10,'(1X,A)') '-----'
      WRITE (10,'(1X,A)') 'X='
      WRITE (10,'(1X,5(F12.8))') (X(I), I=1,N)
      WRITE (10,'(/1X,A,D15.8)') 'F=',F
      DO I=1,NP
          WRITE (10,'(1X,A,I2,A,D15.8)') 'C(',I,')=',C(I)
      END DO
      DO I=1,NQ
          WRITE (10,'(1X,A,I2,A,D15.8)') 'H(',I,')=',H(I)
      END DO

      WRITE (10,'(/1X,A,D15.8)') 'Acurv=',ACURV
      DO I=1,NP
          WRITE (10,'(1X,A,I2,A,D15.8)') 'Bcurv(',I,')=',BCURV(I)
      END DO
      DO I=1,NQ
          WRITE (10,'(1X,A,I2,A,D15.8)') 'Ccurv(',I,')=',CCURV(I)
      END DO

C      Write solution to file
      IF (KLOOP.EQ.0) THEN
          WRITE (11,'(1X,I4,1X,D19.12,1X,L1)')
*          KLOOP,F,FEASIBLE
          WRITE (11,'(5(1X,D13.6))') (X(I),I=1,N)
      ELSE
          IF (RFD.NE.1.D6) THEN

```

## Appendix C: Modified Dynamic-Q Program

```

WRITE (11, '(1X,I4,1X,D19.12,1X,L1,1X,D9.3,1X,D9.3)')
*
      KLOOP,F,FEASIBLE,RELXNORM,RFD
      WRITE (11, '(5(1X,D13.6))') (X(I),I=1,N)
      ELSE
WRITE (11, '(1X,I4,1X,D19.12,1X,L1,1X,D9.3,10X)')
*
      KLOOP,F,FEASIBLE,RELXNORM
      WRITE (11, '(5(1X,D13.6))') (X(I),I=1,N)
      END IF
END IF

C      Write solution to screen
      IF (KLOOP.EQ.0) THEN
        WRITE (*, '(1X,I4,1X,D14.7,1X,L1)') KLOOP,F,FEASIBLE
      ELSE
        IF (RFD.NE.1.D6.AND.FEASIBLE) THEN
          WRITE (*, '(1X,I4,1X,D15.8,1X,L1,1X,D9.3,1X,D9.3)')
*
          KLOOP,F,FEASIBLE,RELXNORM,RFD
        ELSE
          WRITE (*, '(1X,I4,1X,D15.8,1X,L1,1X,D9.3)')
*
          KLOOP,F,FEASIBLE,RELXNORM
        END IF
      END IF

C      Exit do loop here on final iteration
      IF (KLOOP.EQ.KLOOPMAX.OR.RFD.LT.FTOL.OR.RELXNORM.LT.XTOL) THEN
        IF (KLOOP.EQ.KLOOPMAX) THEN
          WRITE(*, '(1X,A)') 'Terminated on max number of steps'
          WRITE(11, '(1X,A)') 'Terminated on max number of steps'
          END IF
        IF (RFD.LT.FTOL) THEN
          WRITE(*, '(1X,A)') 'Terminated on function value'
          WRITE(11, '(1X,A)') 'Terminated on function value'
          END IF
        IF (RELXNORM.LT.XTOL) THEN
          WRITE(*, '(1X,A)') 'Terminated on step size'
          WRITE(11, '(1X,A)') 'Terminated on step size'
          END IF
        WRITE(*, '(1X,A)') ' '
        WRITE(11, '(1X,A)') ' '
        EXIT
      END IF

C*****SOLVE THE APPROXIMATED SUBPROBLEM*****C

      CALL LFOPC77(N,X,NP,NQ,F,C,H,GF,GC,GH,ACURV,BCURV,CCURV,DML,
*
      F_A,C_A,H_A,NL,NU,NLV,NUV,V_LOWER,V_UPPER,xtol,KLOOP)

C      Record solution to approximated problem

      WRITE (10, '(/A)') 'Solution of approximated problem:'
      WRITE (10, '(/1X,A)') 'X='
      WRITE (10, '(1X,5(F12.8))') (X(I), I=1,N)
      WRITE (10, '(/1X,A,D15.8)') 'F_A=',F_A
      DO I=1,NP+NL+NU+N
        WRITE (10, '(1X,A,I2,A,D15.8)') 'C_A(',I,')=',C_A(I)
      END DO
      DO I=1,NQ
        WRITE (10, '(1X,A,I2,A,D15.8)') 'H_A(',I,')=',H_A(I)
      END DO

C      Increment outer loop counter
      KLOOP=KLOOP+1
END DO

C      Write final constraint values to file

WRITE (11, '(/1X,A)') 'Final function value:'
WRITE (11, '(1X,A,D19.12)') 'F=',F

```

## Appendix C: Modified Dynamic-Q Program

```

      IF (NP.GT.0) THEN
        WRITE (11,'(/1X,A)') 'Final inequality constraint
* function values:'
        DO I=1,NP
          WRITE (11,'(1X,A,I2,A,D15.8)') 'C(',I,')=',C(I)
        END DO
      END IF
      IF (NQ.GT.0) THEN
        WRITE (11,'(/1X,A)') 'Final
* equality constraint function values:'
        DO I=1,NQ
          WRITE (11,'(1X,A,I2,A,D15.8)') 'H(',I,')=',H(I)
        END DO
      END IF
      IF (NL.GT.0) THEN
        WRITE (11,'(/1X,A)') 'Final side (lower)
* constraint function values:'
        DO I=1,NL
          WRITE (11,'(1X,A,I2,A,D15.8)') 'C(X(',NLV(I),')='
*           ,C_A(NP+I)
        END DO
      END IF
      IF (NU.GT.0) THEN
        WRITE (11,'(/1X,A)') 'Final side (upper)
* constraint function values:'
        DO I=1,NU
          WRITE (11,'(1X,A,I2,A,D15.8)') 'C(X(',NUV(I),')='
*           ,C_A(NP+NL+I)
        END DO
      END IF

C      Write final X values to screen (DDK 23/11/2000)
      WRITE (*,'(1X,A)') 'Final design variables values:'
      DO I=1,N
        WRITE (*,'(1X,A,I2,A,D15.8)') 'X(',I,')=',X(I)
      ENDDO
      WRITE (*,*)

C      Write final constraint values to screen
      IF (PRNCONST) THEN
        PAUSE 'Constraint values follow: Press enter to continue'
        IF (NP.GT.0) THEN
          WRITE (*,'(/1X,A)') 'Final inequality constraint
* function values:'
          DO I=1,NP
            WRITE (*,'(1X,A,I2,A,D15.8)') 'C(',I,')=',C(I)
          END DO
        END IF
        IF (NQ.GT.0) THEN
          WRITE (*,'(/1X,A)') 'Final
* equality constraint function values:'
          DO I=1,NQ
            WRITE (*,'(1X,A,I2,A,D15.8)') 'H(',I,')=',H(I)
          END DO
        END IF
        IF (NL.GT.0) THEN
          WRITE (*,'(/1X,A)') 'Final side (lower)
* constraint function values:'
          DO I=1,NL
            WRITE (*,'(1X,A,I2,A,D15.8)') 'C(X(',NLV(I),')='
*           ,C_A(NP+I)
          END DO
        END IF
        IF (NU.GT.0) THEN
          WRITE (*,'(/1X,A)') 'Final side (upper)
* constraint function values:'
          DO I=1,NU
            WRITE (*,'(1X,A,I2,A,D15.8)') 'C(X(',NUV(I),')='

```



## Appendix C: Modified Dynamic-Q Program

```

*           ,C_A(NP+NL+I)
          END DO
        END IF
      END IF

      RETURN
    END SUBROUTINE DYNQ77

```

**gradfch77.for**

```

C*****C
C      USER SPECIFIED SUBROUTINE                                C
C      SUBROUTINE GRADFCH(N,X,NP,NQ,GF,GC,GH,F_X,C_X,H_X,DELTX,KLOOP) C
C      COMPUTE THE GRADIENT VECTORS OF THE OBJECTIVE FUNCTION F, C
C      INEQUALITY CONSTRAINTS C, AND EQUALITY CONSTRAINTS H      C
C      W.R.T. THE VARIABLES X(I):                               C
C          GF(I), I=1,N                                         C
C          GC(J,I), J=1,NP I=1,N                               C
C          GH(J,I), J=1,NQ I=1,N                               C
C*****C
      IMPLICIT REAL*8 (A-H,O-Z),INTEGER(I-N)
      DIMENSION X(N),GF(N),GC(NP,N),GH(NQ,N)
      DIMENSION DX(N),C_X(NP),H_X(NQ),C_D(NP),H_D(NQ)
      DIMENSION DELTX(N)

C      Determine gradients by finite difference

      !      DELTX=1.D-5 ! Finite difference interval

      !      CALL FCH(N,NP,NQ,X,F_X,C_X,H_X)
      DO I=1,N
        DO J=1,N
          IF (I.EQ.J) THEN
            DX(J)=X(J)+DELTX(J)
          ELSE
            DX(J)=X(J)
          END IF
        END DO
        CALL FCH(N,NP,NQ,DX,F_D,C_D,H_D,KLOOP,I)
        GF(I)=(F_D-F_X)/DELTX(I)
        DO J=1,NP
          GC(J,I)=(C_D(J)-C_X(J))/DELTX(J)
        END DO
        DO J=1,NQ
          GH(J,I)=(H_D(J)-H_X(J))/DELTX(J)
        END DO
      END DO

      RETURN
    END SUBROUTINE GRADFCH

```

**fch77.for**

```

C*****C
C      USER SPECIFIED SUBROUTINE                                C
C      SUBROUTINE FCH(N,NP,NQ,X,F,C,H,KLOOP,NLOOP)              C

```

## Appendix C: Modified Dynamic-Q Program

```

C
C      COMPUTE OBJECTIVE FUNCTION : F
C      INEQUALITY CONSTRAINT FUNCTIONS : C
C      EQUALITY CONSTRAINT FUNCTIONS : H
C
C
C
C*****
      IMPLICIT REAL*8 (A-H,O-Z),INTEGER(I-N)
      DIMENSION X(N),C(NP),H(NQ)
      integer ios,node
      real time,maktke,tke

C Fluent Simulation (running on lnx86 DDK - 2002)
C Call Pre-processor
      OPEN (33,FILE='parameterset.jou')
      DO i=1,N
         WRITE (33,'(A,I1,A,D20.8)') '$x',i,' = ',X(i)
      END DO
      CLOSE(33)
C Call Gambit
      CALL SYSTEM('gambit_script')
! For windows use the file command below
!   CALL SYSTEM('gambit_script.bat')

C Call Fluent
      CALL SYSTEM('fluent_script')
! For windows use the file command below
!   CALL SYSTEM('fluent_script.bat')
!   Example of what should be in script: fluent 3d -g -wait -i input.jou

C Call Post
      maxtke = 0.
      ! Extract maximum tke from file
      open(99,file='tke.out')
      read(99,*)
      read(99,*)
      read(99,*)
      read(99,*)
      ios=0
      READ (99, *,iostat=ios) time,tke
      DO WHILE (ios.eq.0)
!       Check maximum
         if (tke.gt.maxtke) maxtke=tke
         READ (99, *,iostat=ios) time,tke
      END DO
      close(99)
      F = maxtke

! Move case, data etc. to new file name
      OPEN (33,FILE='move_script')
      WRITE (33,'(A, I2.2, A, I2.2, A)')
      # 'mv groot_impact.cas.gz groot_impact',KLOOP,'_',NLOOP,'.cas.gz'
      WRITE (33,'(A,I2.2,A,I2.2,A)')
      # 'mv groot_impact.dat.gz groot_impact',KLOOP,'_',NLOOP,'.dat.gz'
      WRITE (33,'(A,I2.2,A,I2.2,A)')
      # 'mv tke.out tke',KLOOP,'_',NLOOP,'.out'
      CLOSE(33)
      CALL SYSTEM('chmod u+x move_script')
      CALL SYSTEM('./move_script')
      CALL SYSTEM('rm move_script')

! Constraint
      C(1) = 200. - x(2) + x(3)

      RETURN
      END SUBROUTINE FCH

```

~~~~~

---

## APPENDIX D: GAMBIT JOURNAL FILES FOR IMPACT PAD CREATION AND MESH GENERATION

---

This appendix contains the two Gambit journal files that were used to automatically create the impact pad and mesh the geometry used in Case study 3 of Chapter 4. The first file (gambitsetup.jou) creates the impact pad according to the supplied design variables. The design variables are defined as variables at the start of the journal (e.g. \$l, \$h1 etc). The second file (groot\_opt.jou) imports the impact pad created by the previous file into an existing model of the tundish. The journal file then moves the impact pad to the correct location and does the necessary operations on it, after which the geometry is meshed.

### **gambitsetup.jou**

```
/ Impact pad creation
/ DdK 19/2/2002
/ DdK 13/2/2002 - Added dam at outlet
/ Define paramaters
$w1 = 650.
$w2 = 250.
$l = <<l>>
$h1 = <<h1>>
$h2 = <<h2>>
$d1 = <<d1>>
```

*Appendix D: Gambit Journal Files for Impact Pad Creation*

---

```

$d2 = <<d2>>
$d3 = <<d3>>
$p1 = <<p1>>
$h3 = <<h3>>

volume create width $l depth $h1 height $w1 offset ($l/2.) ($h1/2.) ($w1/2) brick
vertex cmove "vertex.5" multiple 1 offset 50 0 0
vertex cmove "vertex.5" multiple 1 offset 50 (-$h2) 0
vertex cmove "vertex.1" multiple 1 offset 0 130 0
edge create straight "vertex.9" "vertex.10" "vertex.11"
vertex copy "vertex.10"
vertex align "vertex.12" translation "vertex.5" "vertex.6"
coordinate create cartesian vertices "vertex.10" "vertex.11" "vertex.12"
vertex create onedge "edge.14" uparameter 0.5
vertex move "vertex.13" offset 0 0 $d2
edge create nurbs "vertex.10" "vertex.13" "vertex.11" interpolate
edge delete "edge.14" lowertopology
face create translate "edge.13" "edge.15" onedge "edge.8"
coordinate activate "c_sys.1"
vertex cmove "vertex.11" multiple 1 offset 0 0 -50
vertex cmove "vertex.16" multiple 1 offset 0 0 50
vertex cmove "vertex.14" multiple 1 offset 0 0 (($w1-$w2)/2.)
vertex cmove "vertex.10" multiple 1 offset 0 0 (-($w1-$w2)/2.)
edge create straight "vertex.20" "vertex.17"
edge create straight "vertex.19" "vertex.18"
vertex create onedge "edge.22" uparameter 0.5
vertex create onedge "edge.23" uparameter 0.5
coordinate create cartesian vertices "vertex.20" "vertex.17" "vertex.12"
vertex cmove "vertex.21" multiple 1 offset 0 ($d1) 0
coordinate create cartesian vertices "vertex.19" "vertex.18" "vertex.10"
vertex cmove "vertex.22" multiple 1 offset 0 ($d1) 0
coordinate activate "c_sys.1"
edge create nurbs "vertex.19" "vertex.24" "vertex.18" interpolate
edge create nurbs "vertex.20" "vertex.23" "vertex.17" interpolate
face create translate "edge.24" "edge.25" vector 0 200 0
face split "face.8" connected face "face.9"
face split "face.11" connected face "face.10"

```

*Appendix D: Gambit Journal Files for Impact Pad Creation*

---

```

edge delete "edge.23" "edge.22" lowertopology
face delete "face.12" lowertopology
volume create translate "face.8" "face.11" vector 0 -50 0
edge split "edge.6" vertex "vertex.15" connected
edge split "edge.3" vertex "vertex.16" connected
edge split "edge.54" vertex "vertex.36" connected
face create wireframe "edge.9" "edge.6" "edge.18" "edge.39" "edge.43" "edge.55" "edge.12" real
volume create translate "face.22" onedge "edge.44" reverse
volume copy "volume.4"
volume align "volume.5" translation "vertex.42" "vertex.7"
volume create translate "face.4" vector 0 55 0
volume create translate "face.3" vector 50 0 0
volume delete "volume.1" lowertopology
face delete "face.7" lowertopology
vertex create onedge "edge.97" uparameter 0.5
vertex move "vertex.70" offset 0 $d3 0
vertex create edgeints "edge.65" "edge.97" real
vertex create edgeints "edge.97" "edge.85" real
edge create nurbs "vertex.72" "vertex.70" "vertex.71" interpolate
edge create straight "vertex.72" "vertex.71"
face create wireframe "edge.107" "edge.108" real
volume create translate "face.50" onedge "edge.98" reverse
face connect real
edge connect real
vertex connect real
volume unite volumes "volume.2" "volume.3" "volume.4" "volume.5" "volume.6" "volume.7" "volume.8"

edge round "edge.113" radius1 20 radius2 0
edge round "edge.116" radius1 0 radius2 20
edge round "edge.124" "edge.114" "edge.52" "edge.123" "edge.128" "edge.118" "edge.127" "edge.115" "edge.34" "edge.117" "edge.16"
radius1 20
volume blend "volume.2"

/New wall
volume create width 50 depth $h3 height 1000 offset -25 ($h3/2) 400 brick
volume align "volume.3" translation "vertex.8" "vertex.2"
volume move "volume.3" offset (-$p1) 0 0

```

*Appendix D: Gambit Journal Files for Impact Pad Creation*

---

```
export acis "../..../impact.sat" ascii sequencing version "6.0"
abort
```

**groot\_opt.jou**

```
/ Import, move + subtract created Impact Pad
import acis "impact.sat" ascii
vertex create onedge "edge.1392" uparameter 0.5
vertex create onedge "edge.1584" uparameter 0.5
volume align "volume.259" "volume.260" translation "vertex.1267" "vertex.1266" rotation1 \
  "vertex.1260" "vertex.1133" rotation2 "vertex.1253" "vertex.1202"

volume create translate "face.886" onedge "edge.1392" reverse
volume create translate "face.893" onedge "edge.1392"
volume create translate "face.896" onedge "edge.1572" reverse
volume create translate "face.906" "face.914" onedge "edge.1630"
volume subtract "volume.256" volumes "volume.259" "volume.261" "volume.262" \
  "volume.265" "volume.263" "volume.264"
volume subtract "volume.255" volumes "volume.260"

/ Merge complex faces
face merge "face.867" "face.882" "face.951" "face.911"
face merge "face.885" "face.952" "face.903" "face.953"
edge merge "edge.1528" "edge.1515" forced
edge merge "edge.1519" "edge.1608" forced
edge merge "edge.1600" "edge.1583" forced
edge merge "edge.1574" "edge.1620" forced
edge merge "edge.1710" "edge.1714" forced
edge merge "edge.1695" "edge.1690" forced
edge merge "edge.1719" "edge.1720" forced
edge merge "edge.1700" "edge.1683" forced
```

*Appendix D: Gambit Journal Files for Impact Pad Creation*

---

```

edge merge "edge.1527" "edge.1543" "edge.1551" forced
edge merge "edge.1586" "edge.1597" "edge.1592" forced

face merge "face.887" "face.926"
face merge "face.897" "face.927"
face merge "face.877" "face.925"
edge merge "edge.1590" "edge.1636" forced
edge merge "edge.1567" "edge.1635" forced

face merge "face.881" "face.869" "face.871" "face.891"
face merge "face.899" "face.901" "face.873" "face.890"
face merge "face.884" "v_face.971" "face.889" "face.894" "v_face.964" \
"face.898" "face.880" "face.892" "v_face.972" "face.875"
edge merge "edge.1545" "edge.1523" forced
edge merge "edge.1580" "edge.1579" forced
edge merge "edge.1536" "edge.1525" "edge.1538" forced
edge merge "edge.1559" "edge.1549" "edge.1571" forced
edge merge "edge.1729" "edge.1730" forced
edge merge "edge.1727" "edge.1726" forced

face merge "face.507" "face.511"
face merge "face.504" "face.506"
edge merge "edge.946" "edge.941" forced
edge merge "edge.944" "edge.952" forced

/Start Meshing
volume delete "volume.247" lowertopology
blayer create first 8 growth 1.2 total 42.944 rows 4 transition 1 trows 0
blayer attach "b_layer.1" volume "volume.248" face "face.516"
/At inlet
edge mesh "edge.961" "edge.844" successive ratio1 1 intervals 28
edge mesh "edge.842" successive ratio1 1 intervals 20
edge mesh "edge.1450" successive ratio1 1 intervals 15
face mesh "face.438" map pintervals 10 size 30
edge mesh "edge.1450" successive ratio1 1 intervals 15
volume mesh "volume.252" cooper source "face.831" "face.437" "face.522" "face.838" size 30
/Impact pad

```

*Appendix D: Gambit Journal Files for Impact Pad Creation*

```

edge mesh "v_edge.1761" "v_edge.1759" "v_edge.1758" "v_edge.1760" \
  "v_edge.1756" "edge.1569" "v_edge.1757" "edge.1728" "v_edge.1763" \
  "v_edge.1762" successive ratio1 1 size 12
edge mesh "edge.1725" "edge.1682" "v_edge.1753" "edge.1723" "edge.1731" \
  "edge.1686" "v_edge.1751" "edge.1732" "v_edge.1748" "v_edge.1746" \
  "v_edge.1755" "v_edge.1754" "v_edge.1747" "v_edge.1749" "edge.1711" \
  "edge.1718" successive ratio1 1 size 20
edge mesh "edge.1712" "edge.1717" successive ratio1 1 intervals 3
face mesh "face.855" map size 30
face mesh "face.854" map size 30
volume mesh "v_volume.259" tetrahedral size 30
/Inlet region
face mesh "face.412" map pintervals 12 size 20
face mesh "face.411" map pintervals 10 size 20
volume mesh "volume.220" cooper source "face.437" "face.410" size 20
/Middle
edge mesh "edge.1738" "edge.1737" successive ratio1 1 intervals 3
volume mesh "volume.255" submap size 40
/Exit area
edge mesh "edge.1426" successive ratio1 1 intervals 26
volume mesh "volume.248" cooper source "face.816" "face.818" size 30
edge mesh "edge.1514" "edge.1513" "edge.939" "edge.921" "edge.1512" successive ratio1 1 size 5
edge modify "v_edge.1764" backward
edge mesh "v_edge.1765" "v_edge.1764" firstlength ratio1 5 size 7
edge mesh "edge.945" "edge.947" successive ratio1 1 size 7
volume mesh "v_volume.260" tetrahedral size 30
edge mesh "edge.918" successive ratio1 1 intervals 30
volume mesh "volume.257" tetrahedral size 7
face mesh "face.486" map pintervals 30 size 15
volume mesh "volume.216" cooper source "face.487" "face.485" size 15

/BC
physics modify "wall_slag" btype face "face.805" "face.831" "face.816"
physics modify "wall_side" btype face "face.806" "face.813" "face.810" \
  "face.809" "face.808" "face.807" "face.812" "face.804" "face.958" \
  "v_face.966" "v_face.968" "v_face.976" "face.833" "face.843" "face.834"
physics modify "wall_bot" btype face "face.950" "face.959" "face.960" \


```



*Appendix D: Gambit Journal Files for Impact Pad Creation*

---

```
"face.814"  
physics modify "wall_stop_ann" btype face "face.508" "face.503" "face.489" \  
"face.516" "v_face.977" "v_face.978"  
physics modify "tundish_inlet_wall" btype face "face.411" "face.438" \  
"face.412"  
physics modify "SEN_inlet_wall" btype face "face.486" "face.502"  
  
/Export mesh  
export fluent5 "tundish.msh"  
abort
```





---

## APPENDIX E: FLUENT JOURNAL FILE FOR SIMULATION OF TUNDISH WITH IMPACT PAD AND EXTRACTION OF RESULTS

---

This appendix contains the Fluent journal file (fluent\_setup.jou) that was used to automatically set-up the Fluent model after the mesh had been generated automatically in Gambit. The journal also automatically runs the simulation and writes out the appropriate files for the data extraction needed for the optimisation algorithm.

### fluent\_setup.jou

```
;; Read full mesh
f/sbo no yes no no
f/s-t fluent.trn
f/r-c tundish.msh
grid/scale 0.001 0.001 0.001
;; Define models
def/mod/energy yes no no no yes
;; def/mod/visc/ke-rng yes
def/mod/visc/ke yes
/def/mat/cc air liquid-steel yes boussinesq 6975 yes constant 817.3 yes constant 31 yes constant 6.4e-3 no no no yes 0.0001107 no yes
/def/oc/grav yes 0 0 -9.81
/def/oc/ot 1773.15
```

*Appendix E: Fluent Journal File for Simulation of Tundish with Impact Pad and Extraction of Results*

---

```
;; BCs
/def/bc/mfi mass_inlet yes 33.25 no 1823.15 no 0 no yes yes yes no no no yes 5 0.084
/def/bc/wall wall_side 0 no 0 no no no -9000 no no no 0 0.5
/def/bc/wall wall_bot 0 no 0 no no no -6000 no no no 0 0.5
/def/bc/wall wall_slag 0 no 0 no no no -18000 no no yes shear-bc-spec-shear 0 0.5 no 0 no 0 no 0
;; Monitors
/solve/monitors/residual/plot yes
;; Initialise
solve/init/cd/mfi mass_inlet
solve/init/sd z 0
solve/init/if
;; Solution Controls
solve/set/ur/p 0.2
solve/set/ur/mom 0.5
solve/set/ur/t 0.7
solve/set/ur/k 0.6
solve/set/ur/e 0.6
solve/set/ur/d 0.7
solve/set/ur/bf 0.7
;; Steady State
;; 1st Order
solve/iter 300
adapt/aty+ 50 200 0 0 yes
solve/iter 50
adapt/miir no mass-imbalance -0.0001 0.0001
adapt/atr 0 0 0 yes
solve/iter 200
;; 2nd Order
solve/set/ds/p 12
solve/set/ds/mom 1
solve/set/ds/t 1
solve/set/ds/k 1
solve/set/ds/e 1
solve/iter 200
adapt/miir no mass-imbalance -0.0001 0.0001
adapt/atr 0 0 0 yes
solve/iter 500
solve/set/ur/mom 0.4
solve/iter 50
```

---

*Appendix E: Fluent Journal File for Simulation of Tundish with Impact Pad and Extraction of Results*


---

```

;; Post
/plot/plot yes tke.out yes no no tke yes 1 0 0 wall_slag ()
;; Set-up particles
;
; random_eddy num_tries diam
/def/inj/ci injection-0 no yes surface no mass_inlet no yes no 100 0.15 no no no 0 0 -0.7692084 6.9e-6 1823.15 0
/def/mat/cc anthracite alumina yes 3200 yes constant 1680 yes 31 yes
/def/inj/ci injection-1 no yes surface no mass_inlet no yes no 100 0.15 no no no 0 0 -0.7692084 1.65e-5 1823.15 0
/def/inj/ci injection-2 no yes surface no mass_inlet no yes no 100 0.15 no no no 0 0 -0.7692084 2.30e-5 1823.15 0
/def/inj/ci injection-3 no yes surface no mass_inlet no yes no 100 0.15 no no no 0 0 -0.7692084 3.21e-5 1823.15 0
/def/inj/ci injection-4 no yes surface no mass_inlet no yes no 100 0.15 no no no 0 0 -0.7692084 4.52e-5 1823.15 0
/def/inj/ci injection-5 no yes surface no mass_inlet no yes no 100 0.15 no no no 0 0 -0.7692084 6.39e-5 1823.15 0
/def/inj/ci injection-6 no yes surface no mass_inlet no yes no 100 0.15 no no no 0 0 -0.7692084 9.03e-5 1823.15 0
/def/inj/ci injection-7 no yes surface no mass_inlet no yes no 100 0.15 no no no 0 0 -0.7692084 0.000137 1823.15 0
; #steps
/define/models/dpm/tracking/max-steps 100000
; Trap on slag layer
/define/bc/wall wall_slag 0 no 0 no no no -18000 no no no 0 0.5 yes trap no 0 no 0 no 0
; Run particles
/file/stop-t
/file/s-t part.trn
/report/dpm-sample-report injection-7 injection-6 injection-5 injection-4 () outflow () () no
/file/stop-t
;; Write case and data
file/wcd
groot_impact.cas.gz

exit

```

---




---

## APPENDIX F: FORTRAN PROGRAM TO EXTRACT DATA

---

This appendix gives the two Fortran77 programs that were used to extract the data that were written to file during the Fluent simulation. The first program (post.for) extracts the maximum turbulent kinetic energy on the free surface of the molten steel. The second program (post\_part.for) extracts the number of particles that has been trapped on the free surface of the molten steel. These programs are used in conjunction with LS-OPT to automate the optimisation procedure.

### post.for

```

~~~~~
      program ls_opt_post
      !!!
      ! This program takes data from Fluent simulation      !
      ! calculate the response and the give to LSOPT      !
      ! !!!
      ! DDK 1/2002      !
      !!!

      real time,maxk,k
      integer ios
      character*255 line

      maxk = 0.
      ! Extract maximum tke from file
      open(99,file='tke.out')
      read(99,*)
      read(99,*)
      read(99,*)
      read(99,*)
      ios=0
      READ (99, *,iostat=ios) time,k
      DO WHILE (ios.eq.0)
      !      Check maximum
      !      if (k.gt.maxk) maxk=k
      !      READ (99, *,iostat=ios) time,k
      END DO
      close(99)

      ! Echo to standard output
      write(*,*) maxk

      end program ls_opt_post
~~~~~

```

### post\_part.for

```

~~~~~
      program ls_opt_post

```

*Appendix F: Fortran Program to Extract Data*

---

```

!!
! This programs takes data from Fluent simulation      !
! calculate the response and give to LSOPT            !
!   !
! The specific response is the number of particles   !
! trapped   !
!   !
! DDK 7/2002   !
!!

      real perc_trapped
      integer tracked,escaped
      integer ios
      character*255 line,line2,line3

! Extract particles trapped from FLUENT
      open(99,file='part.trn')
      read(99,'(A150)') line
      do while (line.ne.'DPM Iteration ....')
         read(99,'(A150)') line
      enddo
      read(99,'(A150)') line
      read(99,'(A16, I4, A11, I4, A150)') line,
+         tracked,line2,escaped,line3
      close(99)
      perc_trapped=(tracked-escaped)/(1.0*tracked)

      write(*,*) perc_trapped

      end program ls_opt_post

```

---



---

# APPENDIX G: STEADY FLOW RESULTS OF CHOSEN IMPACT PAD DESIGN

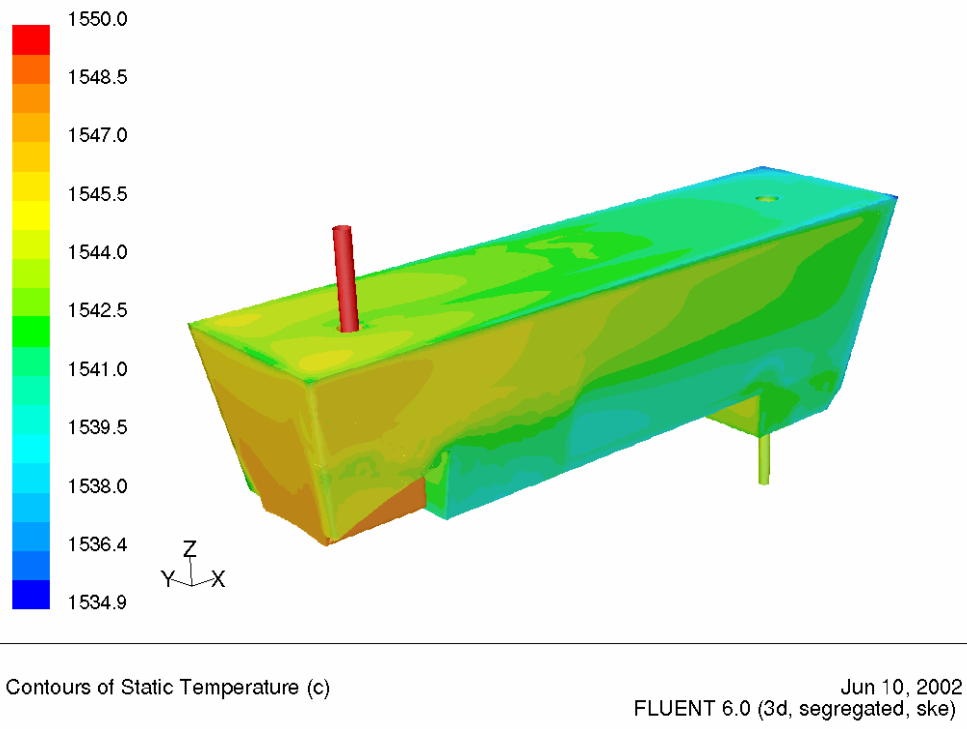
---

## **G-1** INTRODUCTION

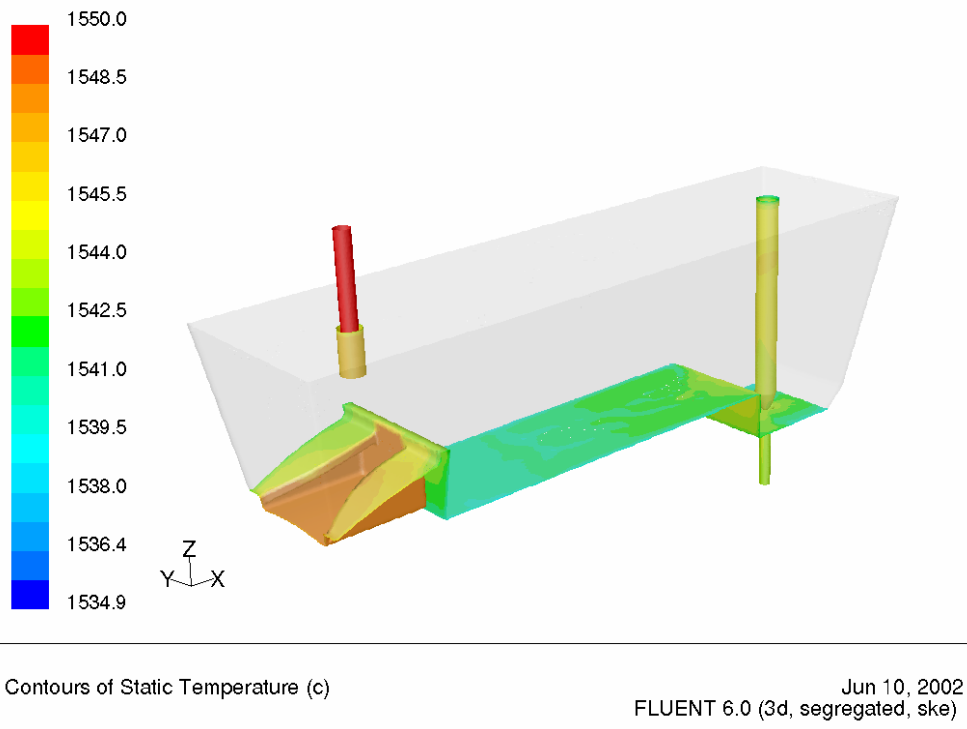
This appendix gives the detail flow results of the optimised impact pad obtained from case study 3. The appendix shows the temperature, flow distribution and turbulence levels in the tundish.

## **G-2** TEMPERATURE CONTOURS

The temperature contours in the tundish are first shown on the walls (Figure G-1 and Figure G-2) and then on vertical planes throughout the tundish width (Figure G-3 through Figure G-7). In Figure G-8, the temperature contours are shown on the slag layer (note that this figure has a reduced scale compared to the other temperature plots, all of which have the same scale). Starting with this last figure, the contours can be seen to be remarkably symmetrical on the slag surface even though the shroud is offset. At the bottom, especially inside the impact pad (Figure G-2), the side wing of the pad nearest the shroud position is notably hotter than the other wing. From the vertical planes (Figure G-3 through Figure G-7), it can be seen that a cold dead zone extends across the whole tundish width in the wake of the impact pad.

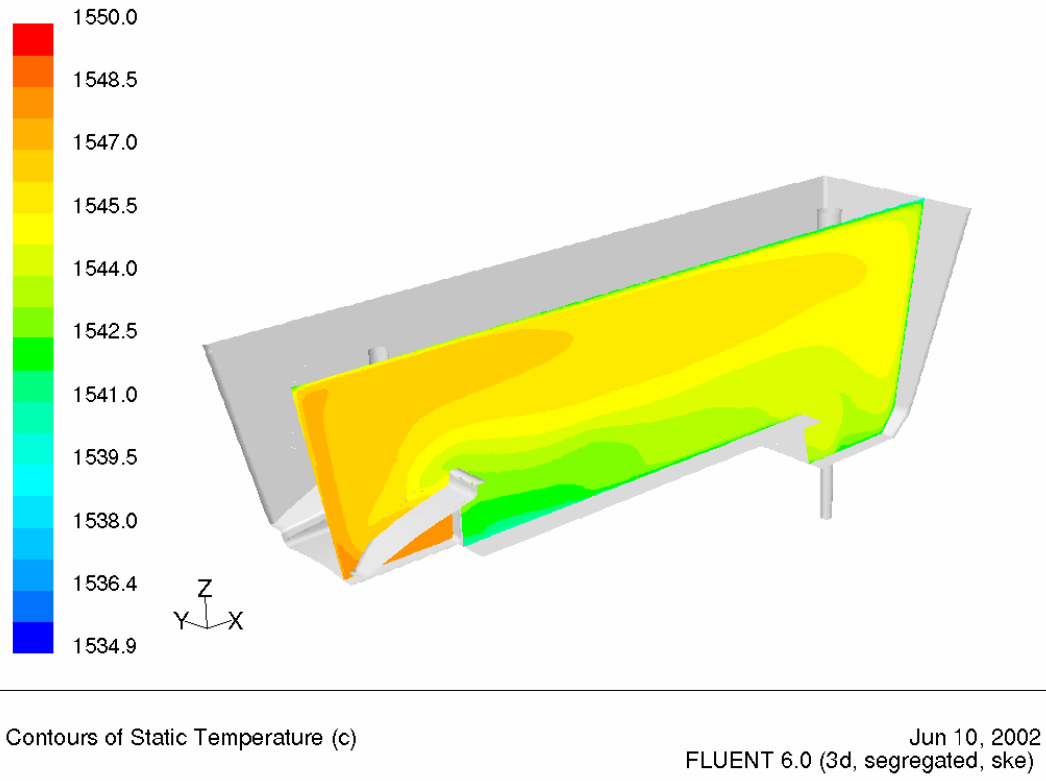


**Figure G-1: Temperature contours on lining**

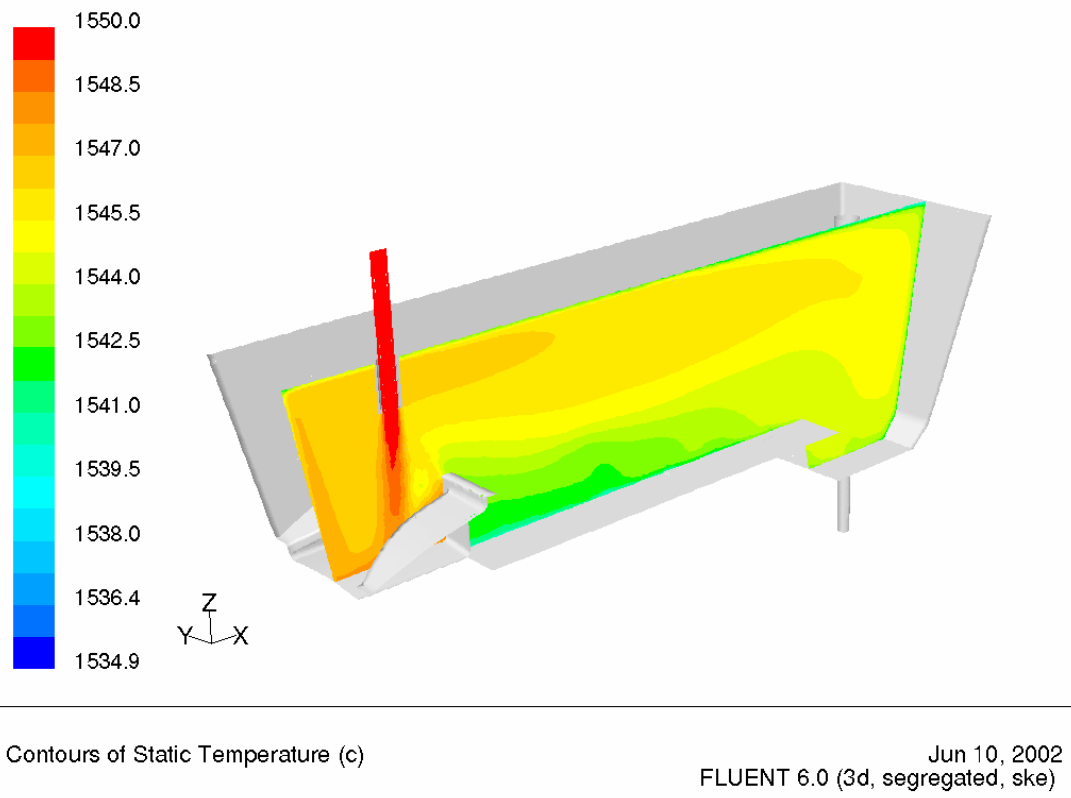


**Figure G-2: Temperature contours on bottom wall and impact pad**

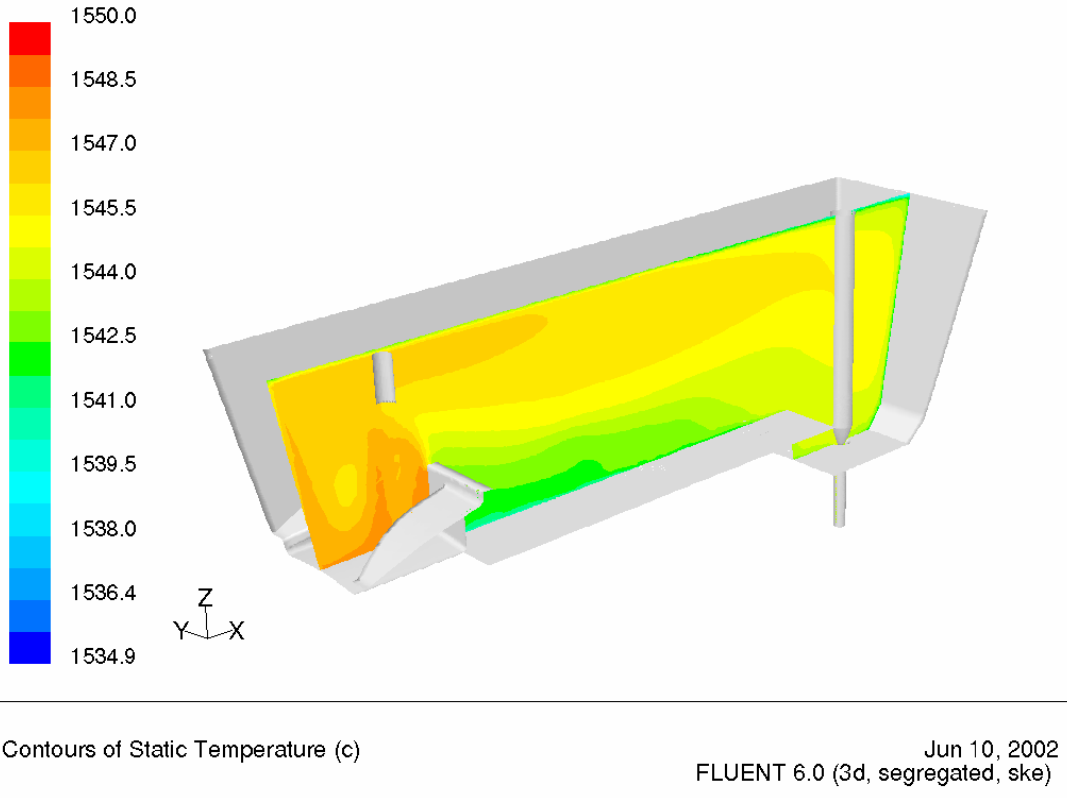




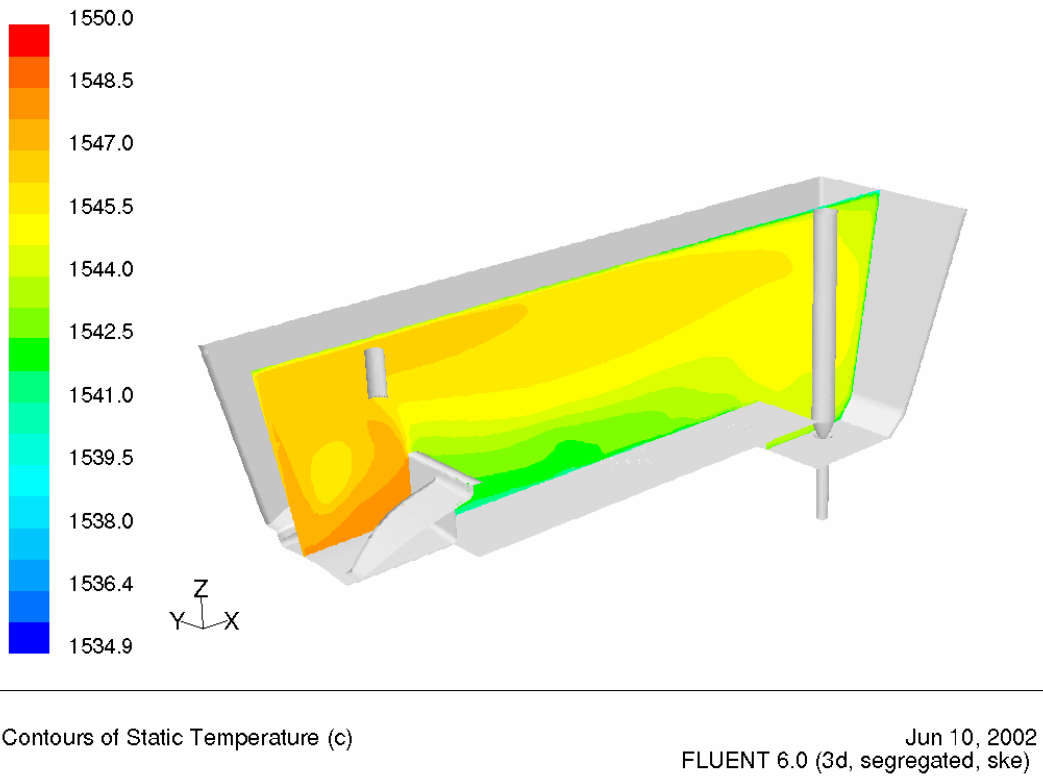
**Figure G-3: Temperature contours on vertical plane – (y=0.2m)**



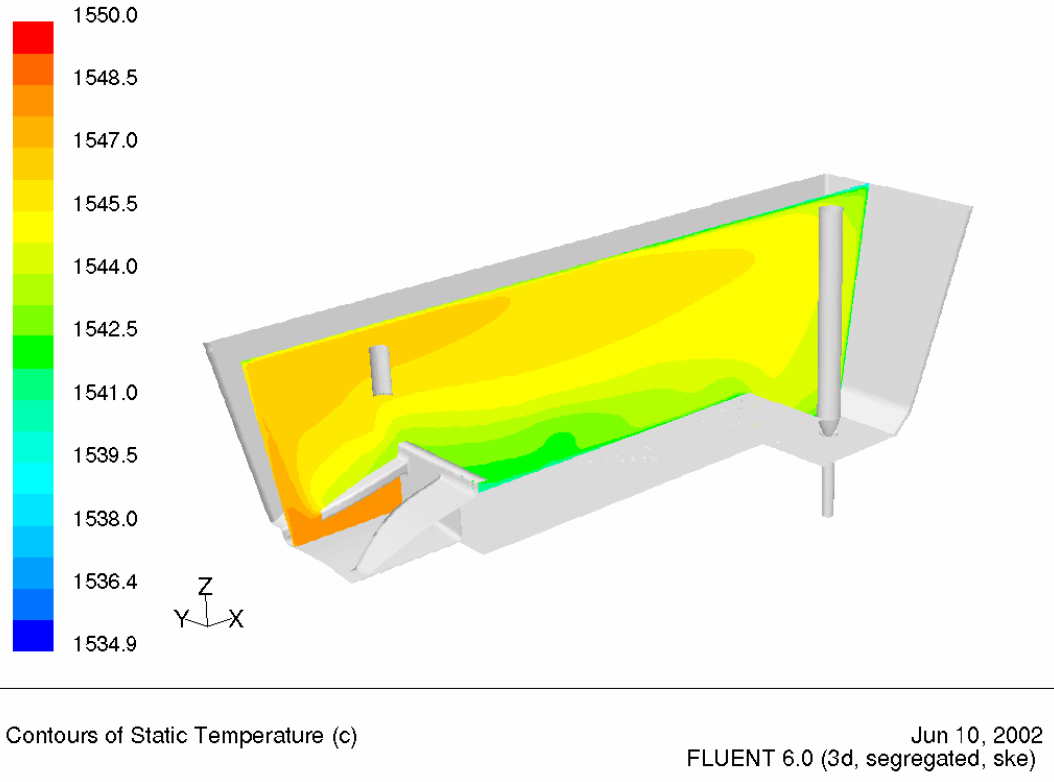
**Figure G-4: Temperature contours on vertical plane – Centre shroud (y=0.32m)**



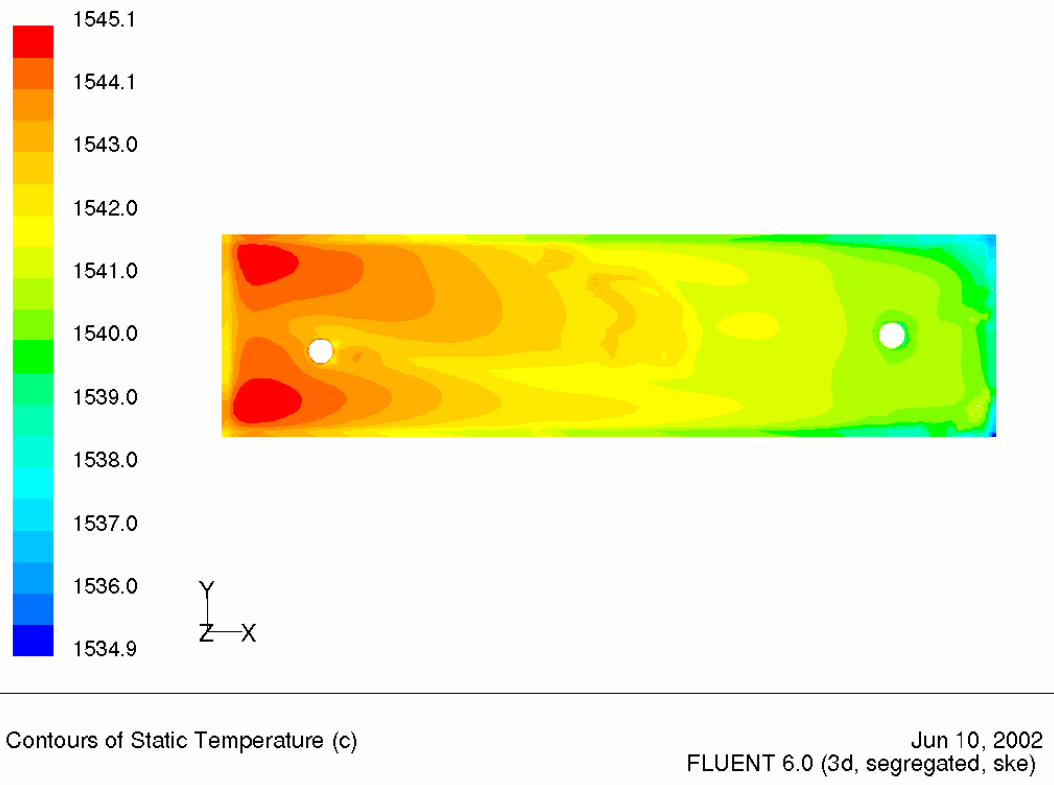
**Figure G-5: Temperature contours on vertical plane – Centre SEN (y=0.4m)**



**Figure G-6: Temperature contours on vertical plane – (y=0.48m)**



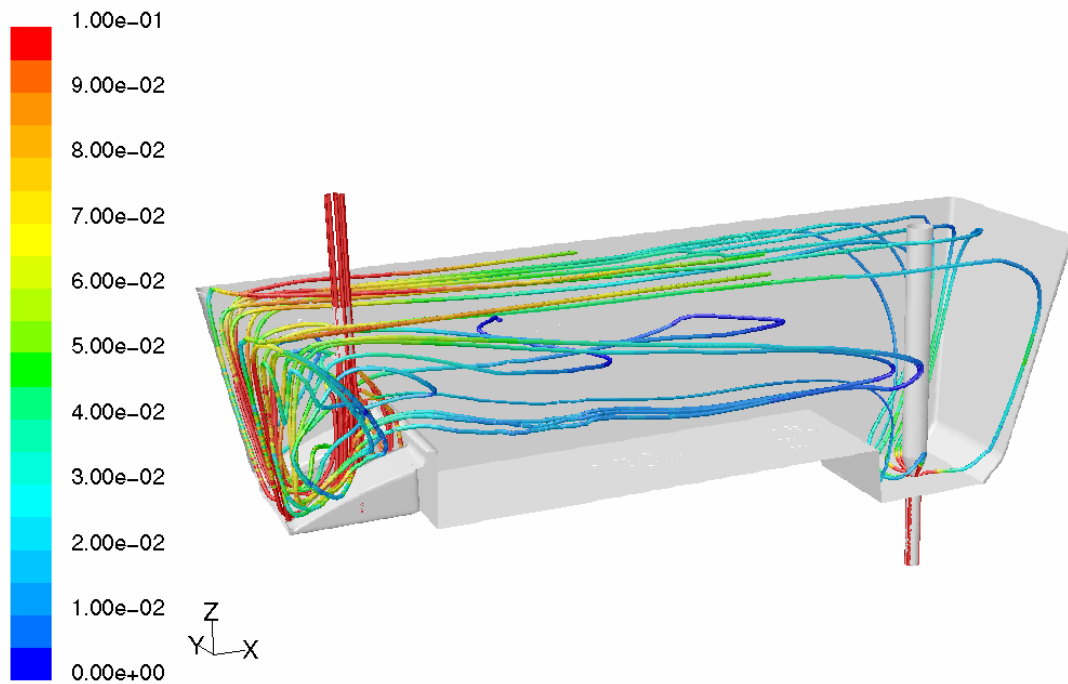
**Figure G-7: Temperature contours on vertical plane – (y=0.6m)**



**Figure G-8: Temperature contours on slag layer**

### G-3 PATH LINES AND CONTOURS OF VELOCITY MAGNITUDE

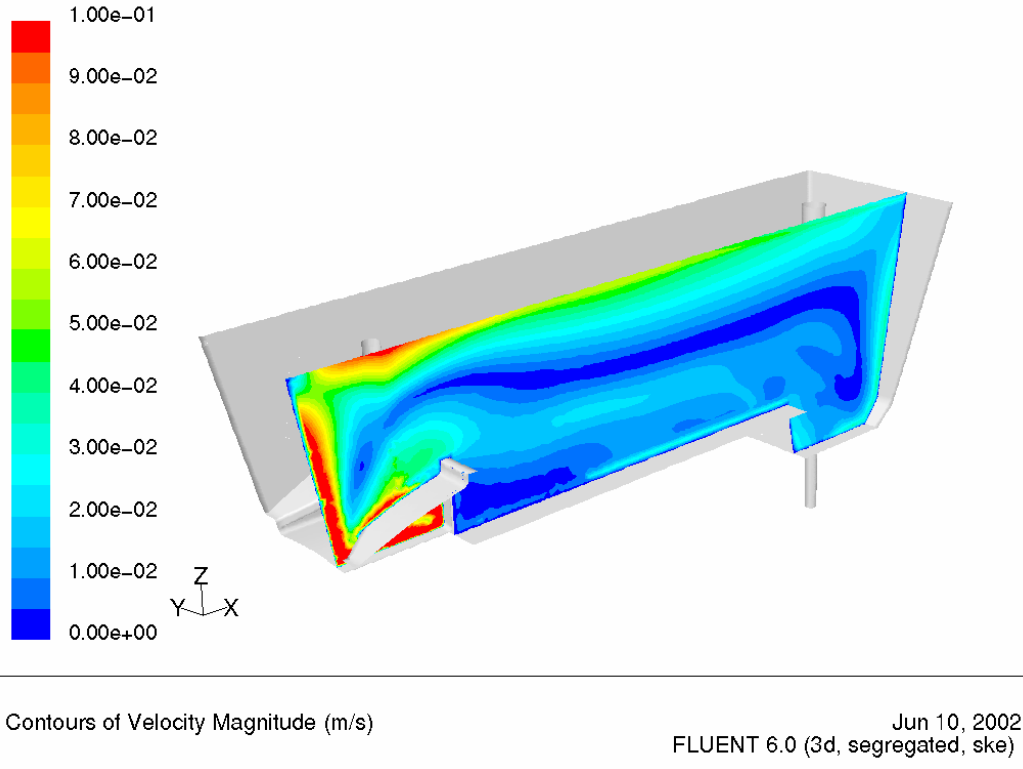
The path lines and contours of velocity magnitude in the tundish on vertical and horizontal planes are shown in Figure G-9 and Figure 10 through Figure G-20 respectively. All contour plots are clipped at  $0.1\text{m}\cdot\text{s}^{-1}$ . Note how the inlet jet is split into two. The one section continues up the back wall and extends along nearly the whole of the length of the tundish just below the slag layer. The other part of the jet forms a 'tongue' that is located at a median height in the tundish. This tongue is fairly two-dimensional in that it extends across the full width of the tundish. There is some evidence of three-dimensional flow due to the off-set shroud, but the impact pad does manage to limit the three-dimensionality of the flow.



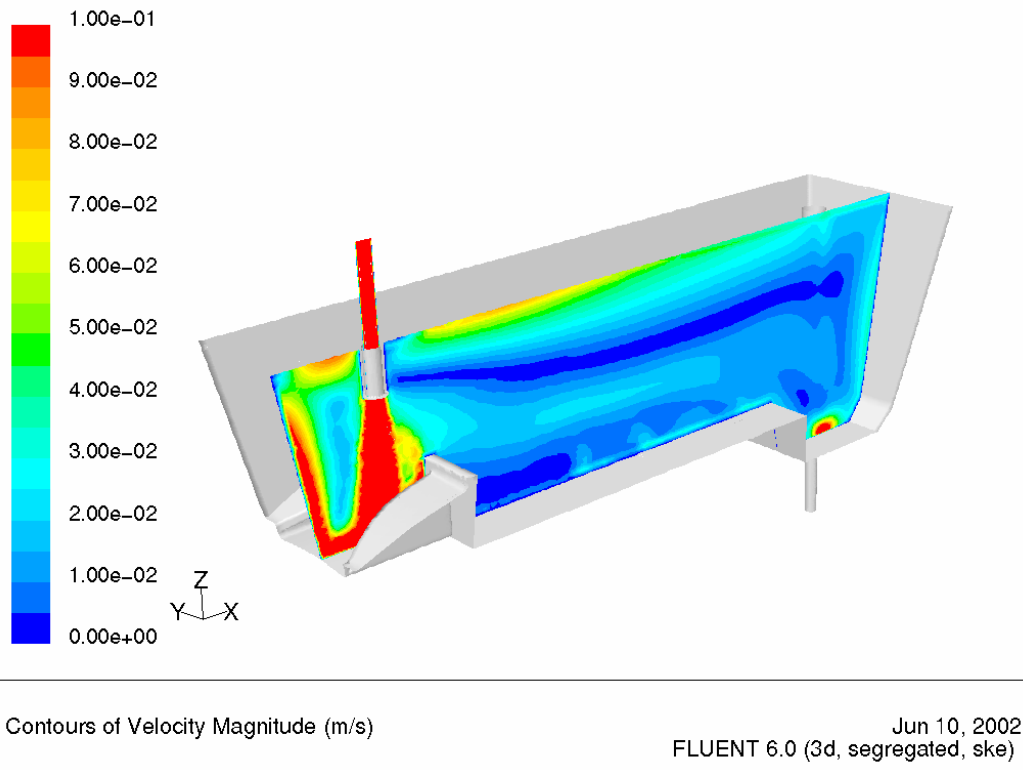
Path Lines Colored by Velocity Magnitude (m/s)

Jun 10, 2002  
FLUENT 6.0 (3d, segregated, ske)

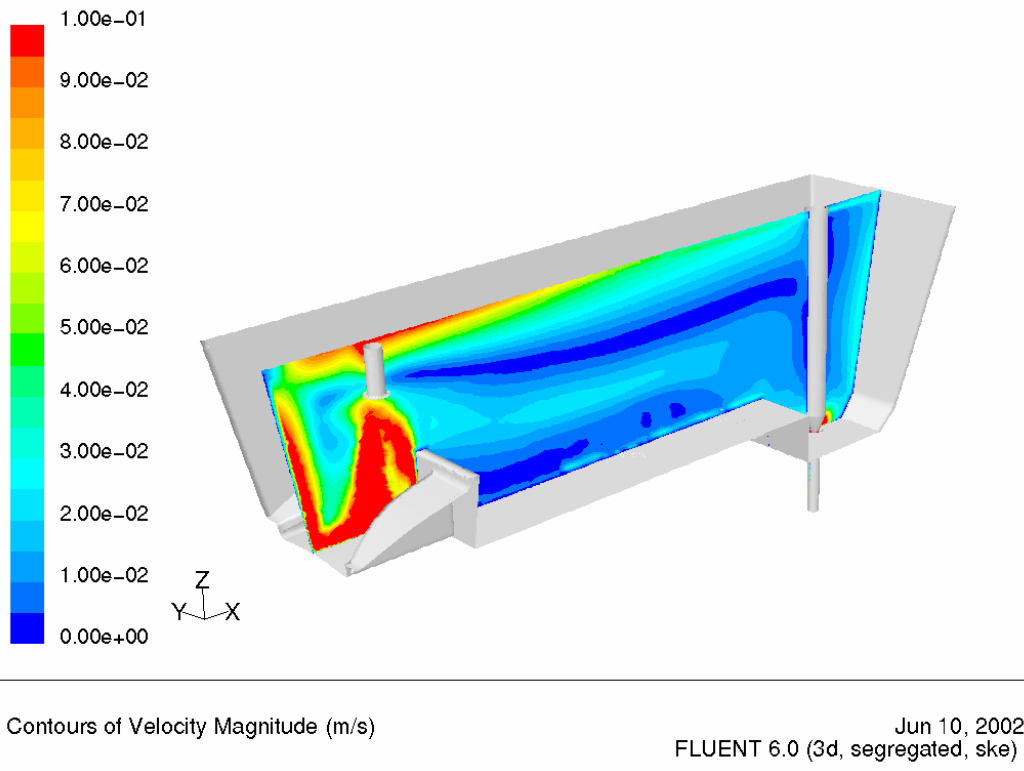
**Figure G-9: Path lines in tundish coloured by velocity magnitude**



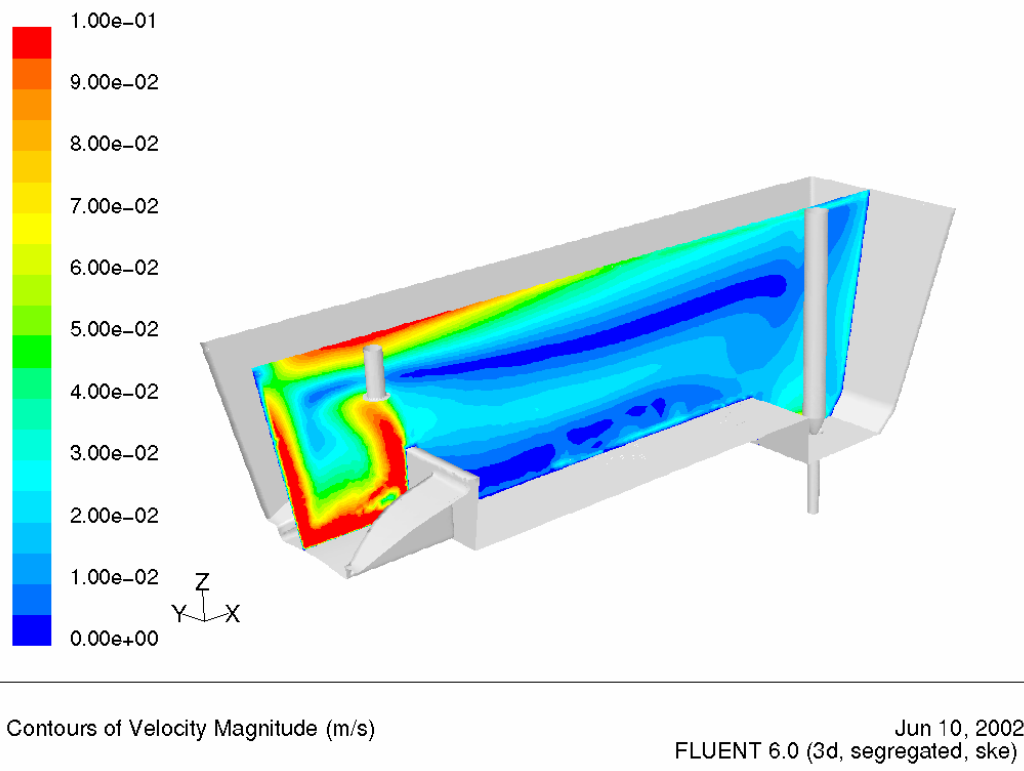
**Figure 10: Velocity magnitude contours on vertical plane – (y=0.2m)**



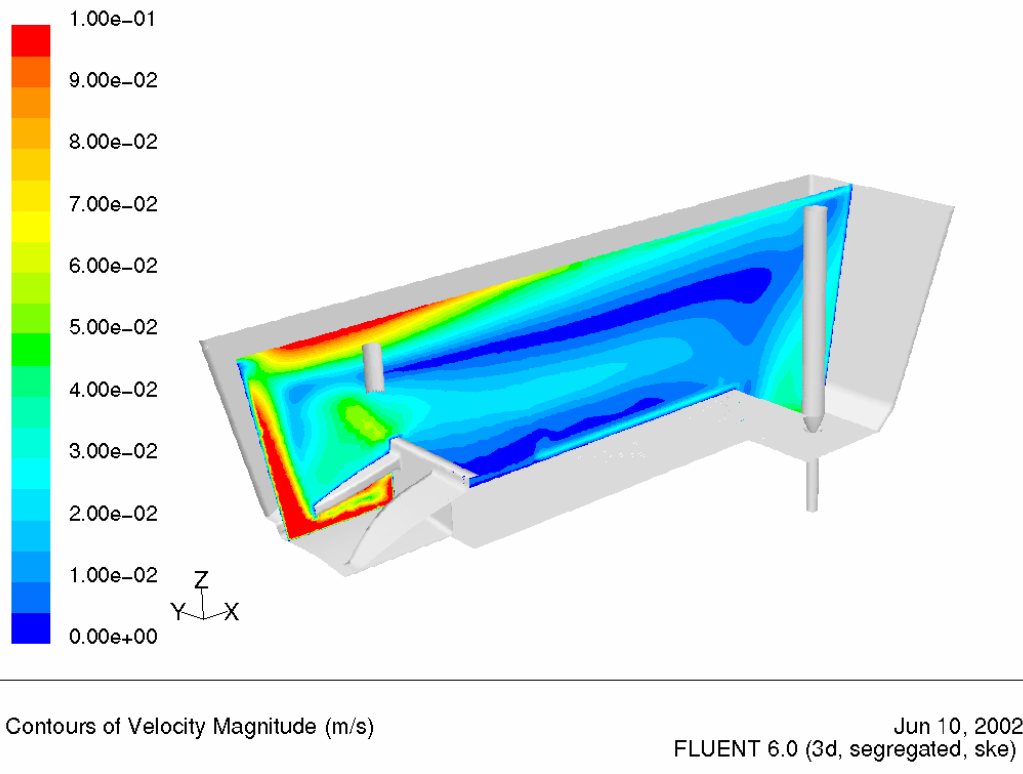
**Figure G-11: Velocity magnitude contours on vertical plane – Centre shroud (y=0.32m)**



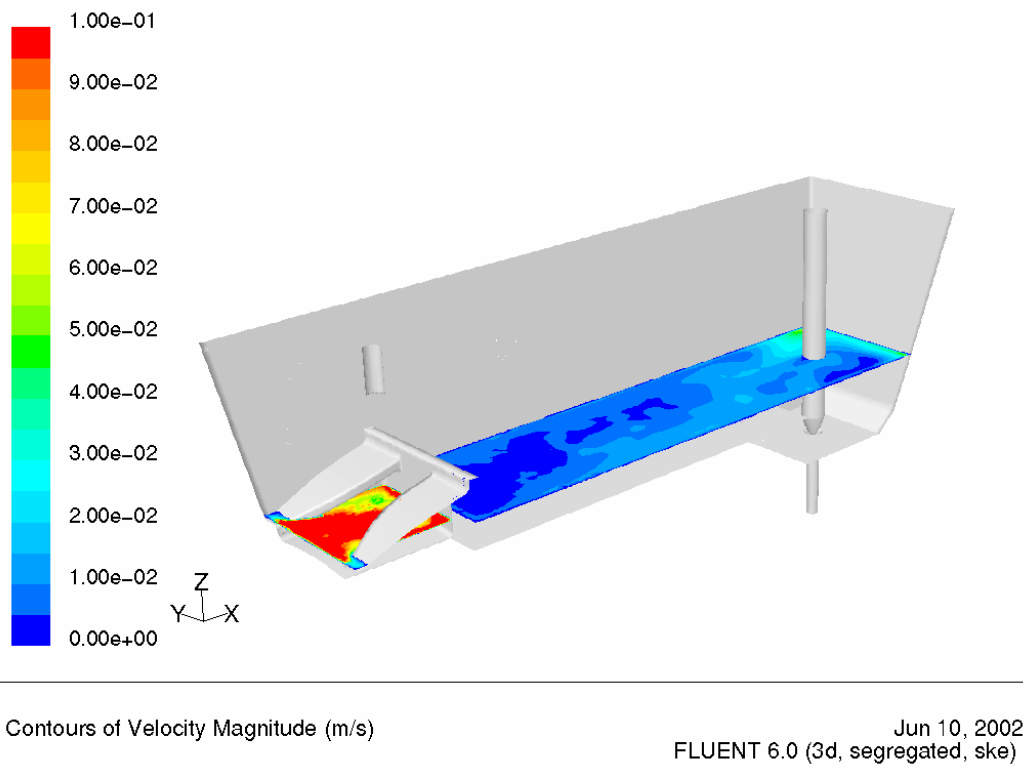
**Figure G-12: Velocity magnitude contours on vertical plane – Centre SEN  
( $y=0.4\text{m}$ )**



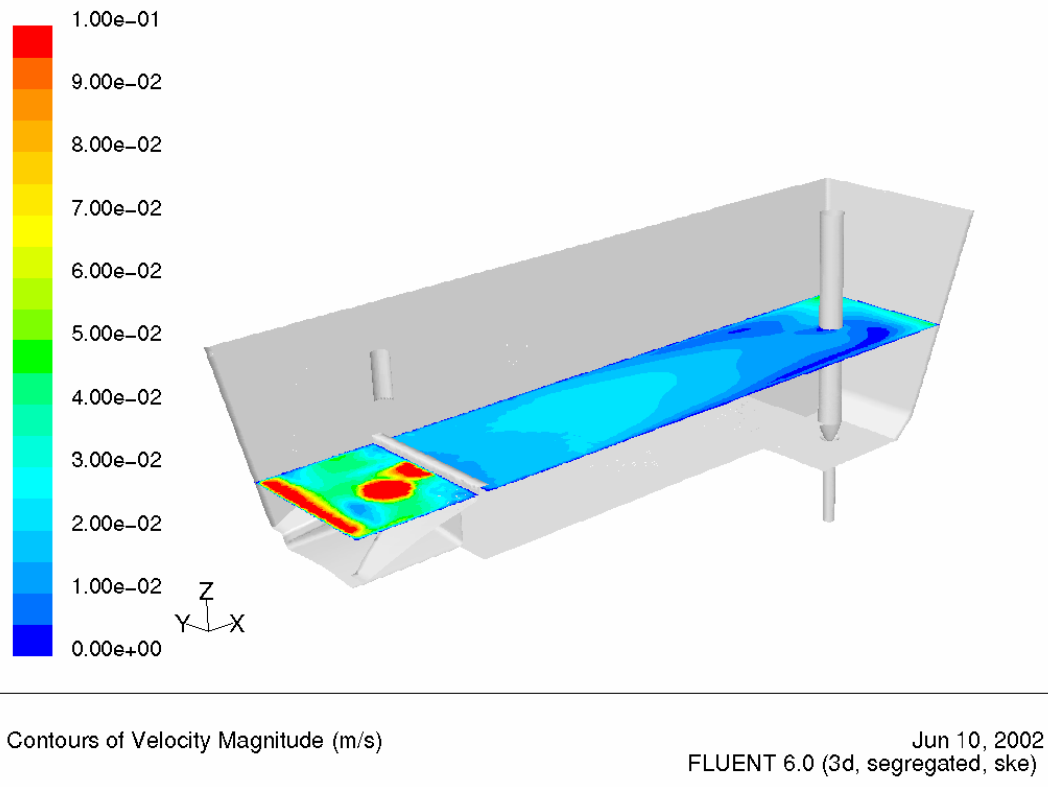
**Figure G-13: Velocity magnitude contours on vertical plane – ( $y=0.48\text{m}$ )**



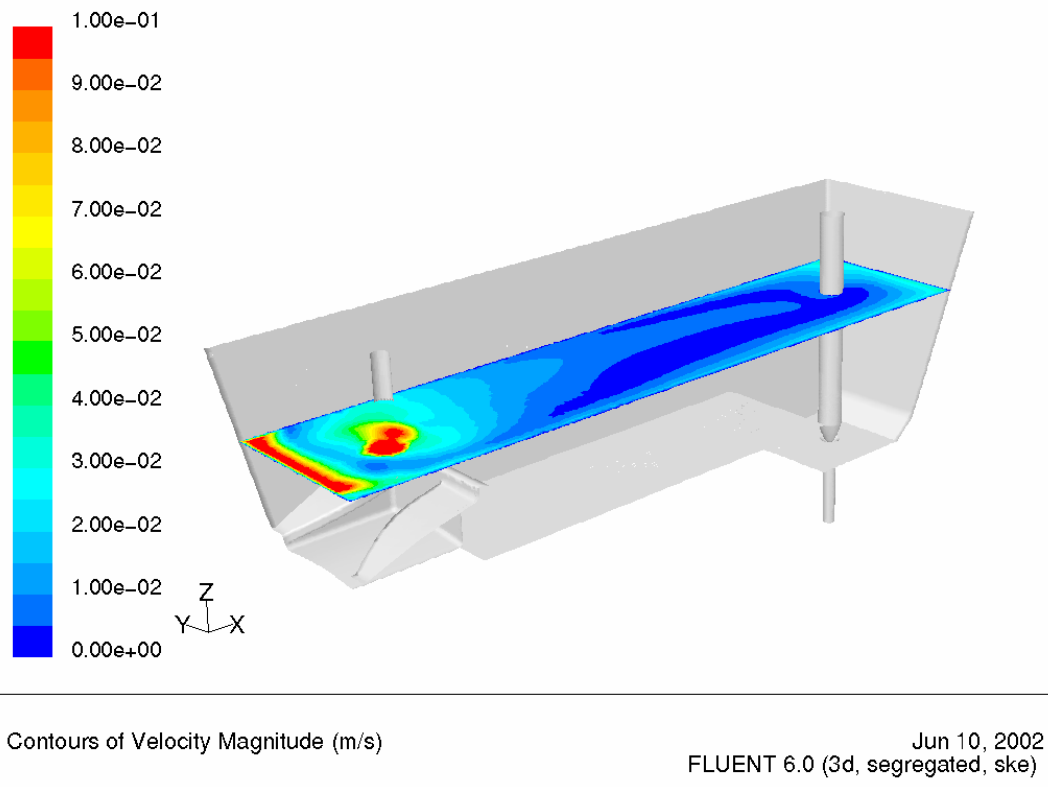
**Figure G-14: Velocity magnitude contours on vertical plane – ( $y=0.6\text{m}$ )**



**Figure G-15: Velocity magnitude contours on horizontal plane – ( $z=-0.6\text{m}$ )**

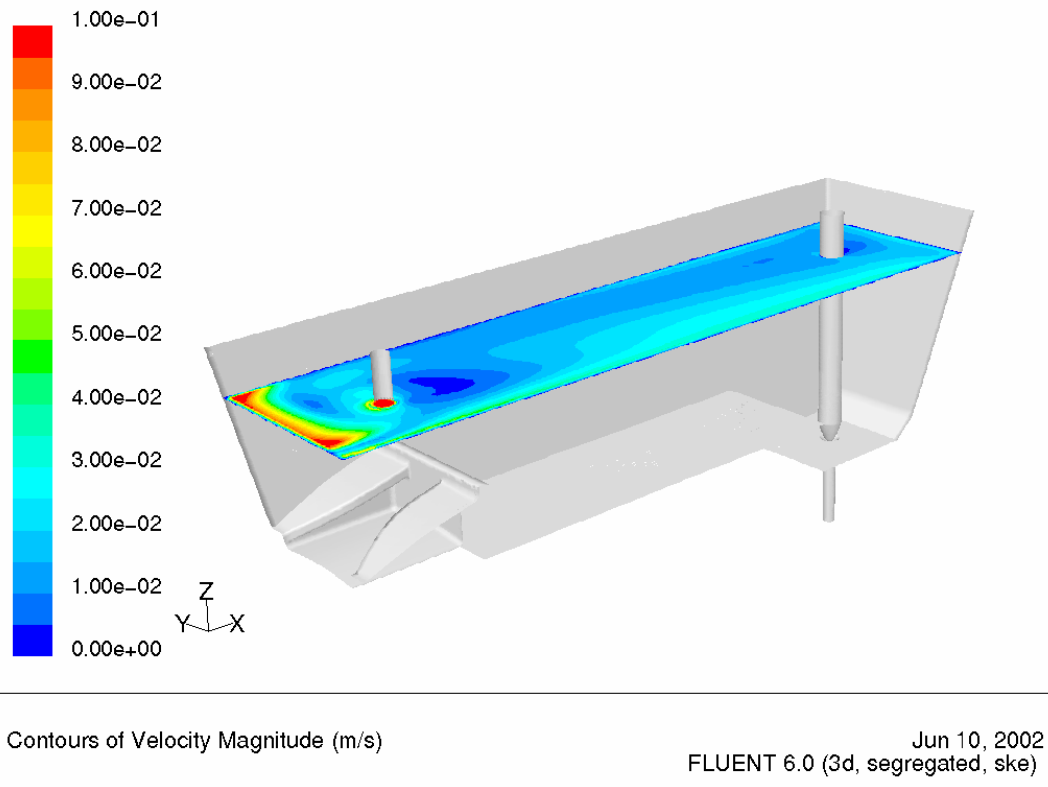


**Figure G-16: Velocity magnitude contours on horizontal plane – (z=-0.4m)**

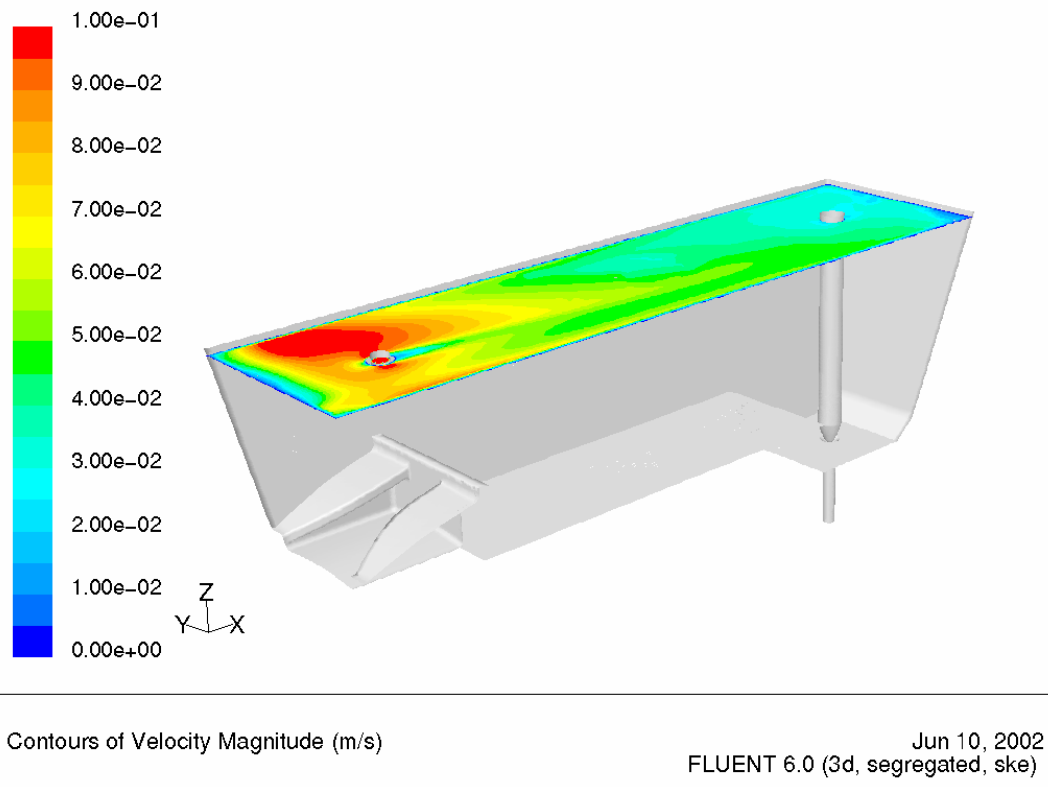


**Figure G-17: Velocity magnitude contours on horizontal plane – (z=-0.2m)**

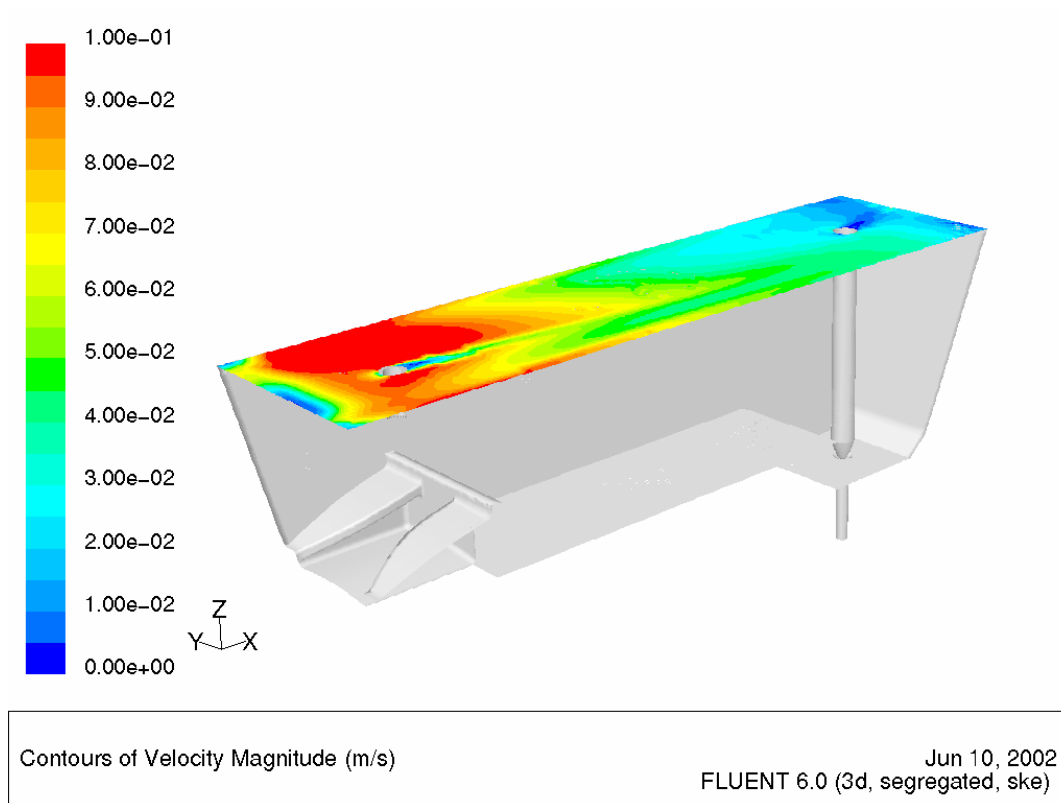




**Figure G-18: Velocity magnitude contours on horizontal plane – (z=0.0m)**



**Figure G-19: Velocity magnitude contours on horizontal plane – (z=0.2m)**



**Figure G-20: Velocity magnitude contours on slag layer**

#### **G-4 TURBULENT KINETIC ENERGY (TKE)**

As the wall TKE can relate to erosion of the refractory, its contours are plotted on all the walls in Figure G-21 and Figure G-22. Note the high levels of TKE on the back wall.

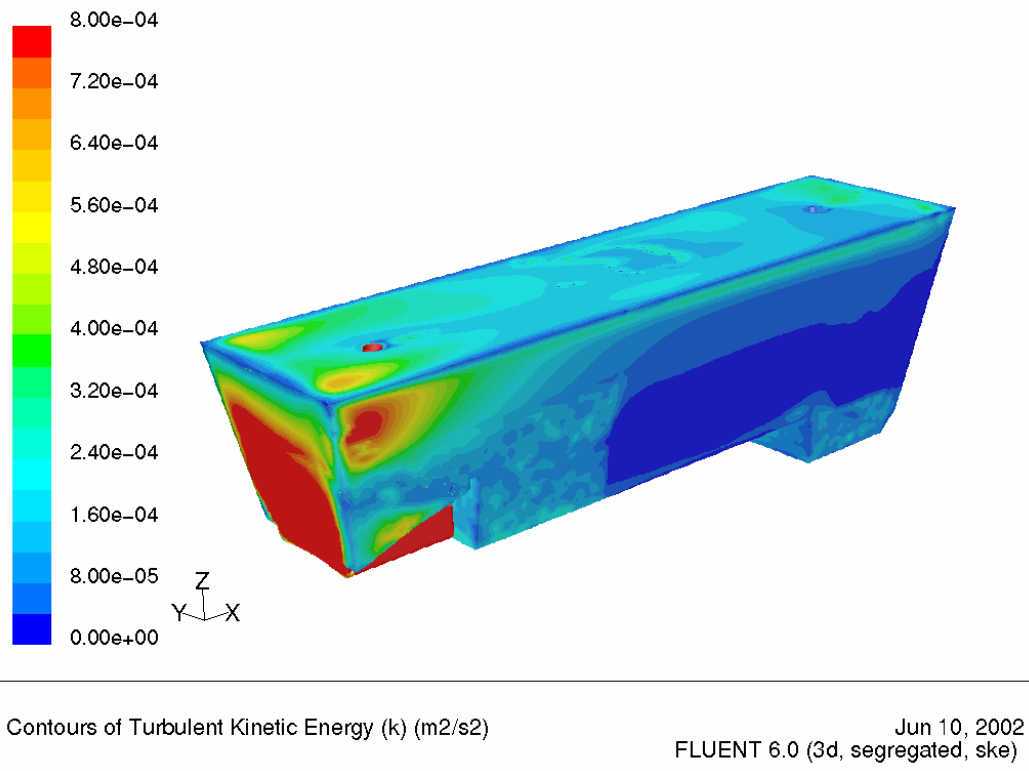


Figure G-21: Wall turbulent kinetic energy contours (front)

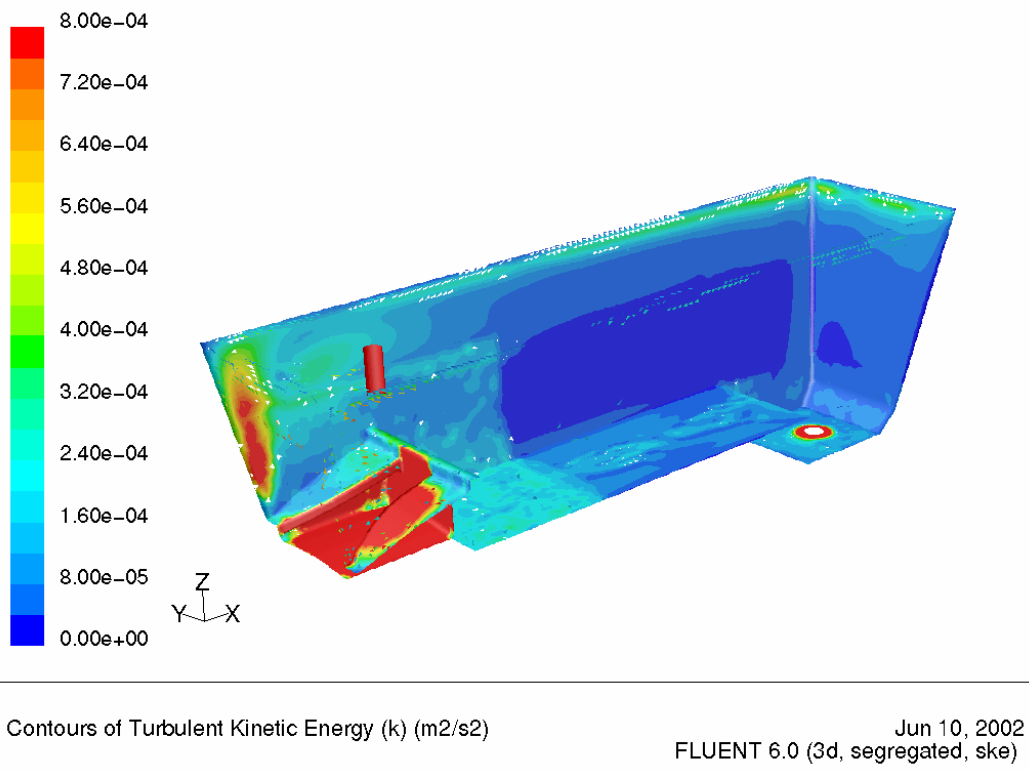
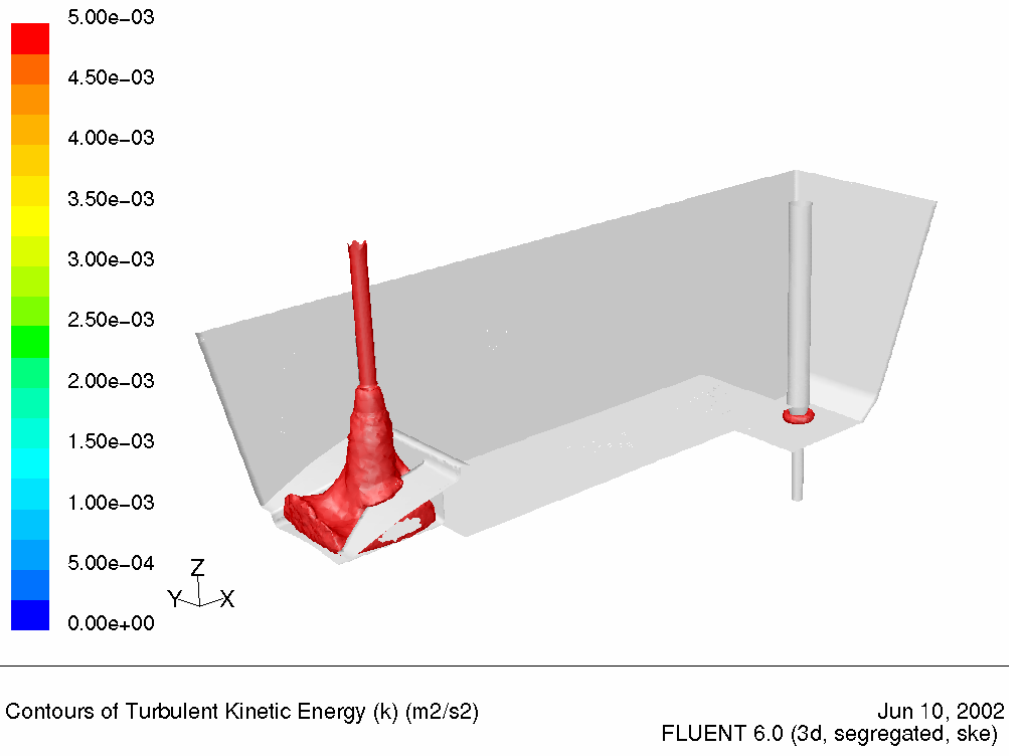
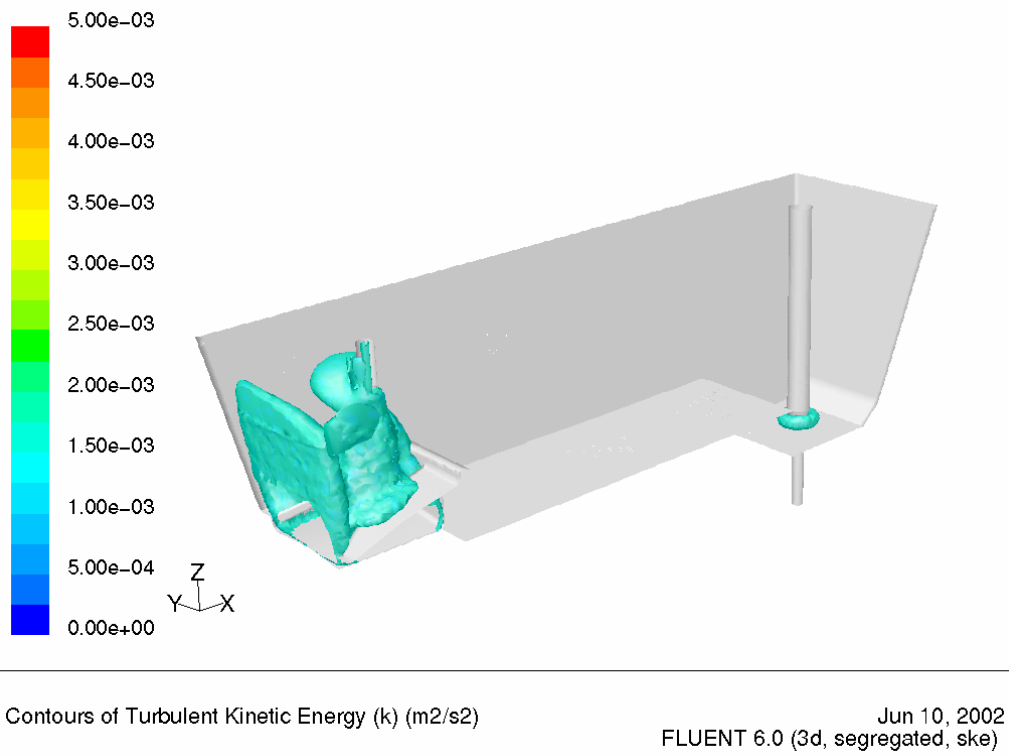


Figure G-22: Wall turbulent kinetic energy contours (back)

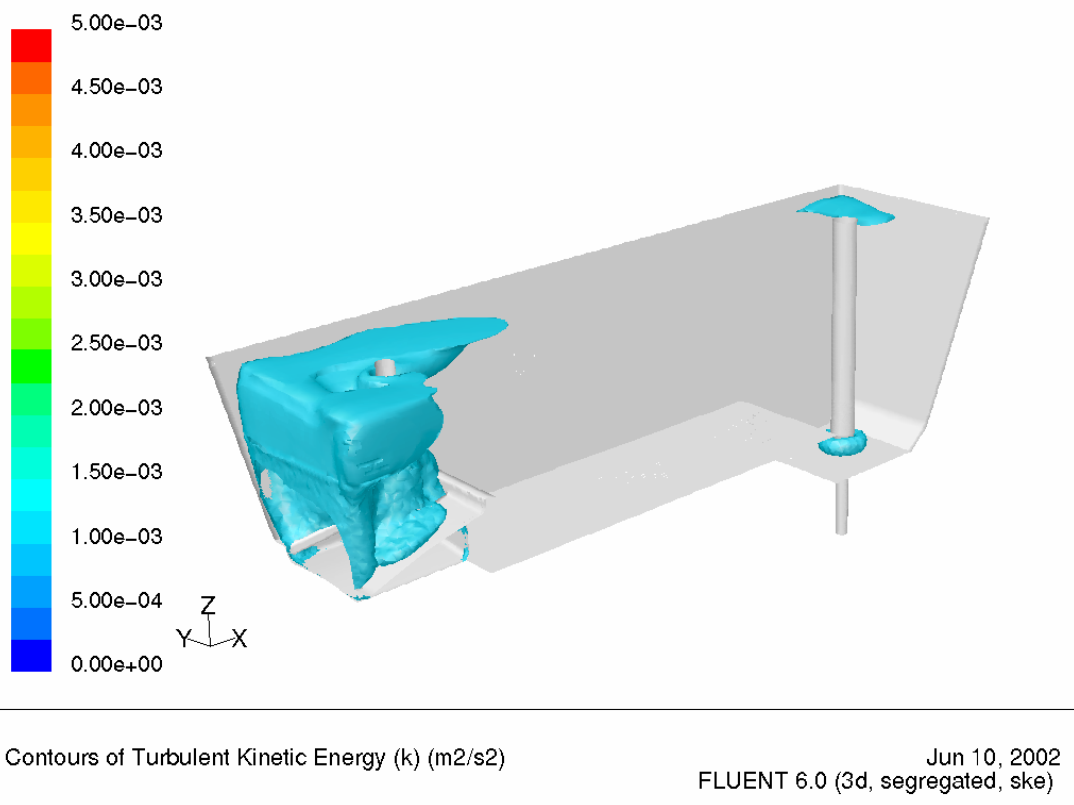
Another view of the TKE performance can be seen from selected iso-surfaces as depicted in Figure G-23 through Figure G-25 for three TKE levels.



**Figure G-23: Iso-surface of turbulent kinetic energy (TKE =  $5 \times 10^{-3} \text{ m}^2 \cdot \text{s}^{-2}$ )**



**Figure G-24: Iso-surface of turbulent kinetic energy (TKE =  $1.5 \times 10^{-3} \text{ m}^2 \cdot \text{s}^{-2}$ )**



**Figure G-25: Iso-surface of turbulent kinetic energy (TKE =  $1 \times 10^{-3} \text{ m}^2 \cdot \text{s}^{-2}$ )**



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## APPENDIX H: PARTICLE TRAPPING USER DEFINED FUNCTION

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This appendix contained the first attempt of a more advanced model for the trapping of a particle on the slag layer. This is a C-program that is compiled as a User Defined Function in Fluent. The model calculates the maximum continuous time that a particle spends in a user defined region close to the slag layer. A simple correlation is then used that relates the probability of a particle being trapped to the size of the particle and the time it spent near the slag layer.

```
/******  
/*UDF for computing the maximum cont. time spent by a particle in the */  
/* region close to the slag layer */  
/* This model assumes: */  
/* z is pointing upwards */  
/* Model inputs: */  
/* thickness of trapping zone */  
/* z-position of slag layer */  
/* */  
/* File History: */  
/* DdK 12/2001 */  
/* DdK 4/2002 Automating output of number trapped */  
/* */  
/******
```

*Appendix H: Particle Trapping User Defined Function*

---

```

#include "udf.h"
#include "sg.h"
#include "dpm.h

static int flag_inzone;
static int num_trapped;
#define thickness 0.002          /* Thickness that slaglayer's effect into steel */
#define top 0.23                /* z-coordinate of the top of the surface */
#define timefact 0.75          /* Time constant used to determine if trapped */

DEFINE_INIT(tsns_setup, domain)
{
    /* Allocate particle variables if not been set */
    if (NULLP(user_particle_vars)) Init_User_Particle_Vars();
    /* Set name and lable */
    strcpy(user_particle_vars[0].name, "time-spent");
    strcpy(user_particle_vars[0].label, "Continuous Time Spent at Surface");
    strcpy(user_particle_vars[1].name, "max-time-spent");
    strcpy(user_particle_vars[1].label, "Max. Continuous Time Spent at Surface");
}

DEFINE_DPM_SCALAR_UPDATE(time_spent, cell, thread, initialise, p)
{
    FILE *fp;

    cphase_state_t *c = &(p->cphase);
    if (initialise)
    {
        /* Initialization call */
        flag_inzone = 0;
        p->user[0] = 0;
        p->user[1] = 0;
    }
    else
    {
        /* Calculate time spent in trapping zone (user[0]) and assign to user[1] if longer than current user[1]*/
        if (p->state.pos[2]>(top-thickness) && p->state.pos[2]<(top+thickness))

```

### Appendix H: Particle Trapping User Defined Function

---

```

        {
            flag_inzone = 1;
            p->user[0] += P_DT(p);
        }
        else if (flag_inzone)
        {
            if (p->user[0]>p->user[1]) p->user[1]=p->user[0]; /* Check if bigger than current max time */
            flag_inzone = 0; /* Reset flag */
            p->user[0] = 0; /* Reset counter */
        }
        /*fp = fopen("output.txt","a");
        fprintf(fp, "%f %f %f %f\n", p->state.pos[0], p->state.pos[1], p->user[0], p->user[1]);
        fclose(fp); */
    }
}

DEFINE_DPM_OUTPUT(time_spent_output, header, fp, p, thread, plane)
{
    /* Post-processing of particle data */
    char name[100];

    if (header)
    {
        num_trapped = 0;
        if (NNULLP(thread))
            fprintf(fp, "(%s %d)\n", thread->head->dpm_summary.sort_file_name, 11);
        else
            fprintf(fp, "(%s %d)\n", plane->sort_file_name, 11);
        fprintf(fp, "(%10s %10s %10s %10s %10s %10s %10s %10s %10s %10s %10s %s)\n",
            "X", "Y", "Z", "U", "V", "W", "diameter", "T", "mass-flow",
            "time", "max-time-spent", "name");
    }
    else
    {
        sprintf(name, "%s:%d", p->injection->name, p->part_id);
        fprintf(fp, "((%10.6g %10.6g %10.6g %10.6g %10.6g %10.6g %10.6g %10.6g %10.6g %10.6g %10.6g %s)\n",
            "%10.6g %10.6g %10.6g %10.6g) %s)\n",

```



*Appendix H: Particle Trapping User Defined Function*

---

```
        p->state.pos[0], p->state.pos[1], p->state.pos[2],
        p->state.V[0], p->state.V[1], p->state.V[2],
        p->state.diam, p->state.temp, p->flow_rate, p->state.time,
        p->user[1], name);
if (p->user[1] >(timefact*p->state.diam*1e6))
{
    num_trapped = num_trapped + 1;
    printf("Particle %s leaving %s would have been trapped \n", name,thread->head->dpm_summary.sort_file_name);
    printf("Total number trapped in trapping zone = %d \n",num_trapped);
}
}
```