LARGE-EDDY SIMULATIONS OF RECIRCULATION ZONES IN CHANNEL-TYPE MOLTEN SALT REACTORS

BY

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THESIS

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Abstract

In an effort to curb carbon emissions and mitigate the effects of climate change, energy policymakers are considering advanced nuclear reactors as a potential source of clean base-load energy. Once such family of reactor designs is called the Molten Salt Reactor, which has been successfully demonstrated experimentally during the operation of the Molten Salt Reactor Experiment (MSRE) at the Oak-Ridge National Laboratory during the 1960s. Thermal-hydraulic simulations of this reactor are an important step towards validating and verifying simulation tools for other molten salt reactor designs and exploring the potential of such reactors for licensing. Modern CFD simulations of the MSRE reactor core often discount the effects of turbulence in this reactor due to the low Reynolds number inside the MSRE channels. They also neglect the pyramidal tip at the top of the moderator graphite blocks called stringers. However, recent research indicates turbulence can play a significant role in compact reactor cores at relatively low Reynolds numbers. Our main concern is entrainment of fuel salt in recirculation zones and subsequent creation of localised hotspots. Therefore, we investigated the presence of such recirculation zones and the effect of the tip-shape on turbulence and stationary vortices in the upper plenum.

We analysed the flow around an MSRE graphite stringer using large eddy simulations performed in Nek5000. We also studied the effects of varying the size and shape of the stringer-tip using Nek5000’s mesh deformation capabilities. To our knowledge, this work is the first effort to apply large eddy simulations to the MSRE and study the effects of geometry-induced turbulence and recirculation within the MSRE. We analysed the output data and found that salt recirculation vortices do exist and geometry and turbulence affect the salt flow in the upper plenum. But fuel salt recirculation does not impact the temperature of the salt or graphite significantly. We also determined the ideal tip-shape that minimises salt recirculation and entrapment. We found that a pyramidal tip with an apex half-angle of 45° disrupts recirculation, encourages mixing, and improves heat transfer, keeping salt and graphite temperatures low, whereas angles that are as small as 30° or large enough to tend towards a flat-top lead to hotter temperatures. Implications for the design and simulation of similar channel-type molten salt reactors are discussed.
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Chapter 1

Introduction

The objective of this thesis is to analyse the flow inside channel-type liquid-fuelled Molten Salt Reactor (MSR)\(s\) [1] (Figure 1.1) using high-fidelity Computational Fluid Dynamics (CFD) to assess the impact of recirculation zones formed in the upper plenum due to flow separation. While experimental data and thermal-hydraulic models aimed at investigating turbulence in MSRs are sparse, there is limited evidence that suggests turbulent behaviour can be observed at relatively low Reynolds numbers in MSRs and vortices formed due to flow separation in MSR plena could entrain fuel salt. Fuel salt that is trapped and recirculating in these zones could create localised hotspots. We investigated the presence of these vortices using Large Eddy Simulation (LES) to obtain a more detailed picture of the turbulence in the upper plenum and to improve upon the existing MSR CFD studies that typically use Reynolds-Averaged Navier Stokes (RANS). Additionally, we also examined the role of geometry in generating these vortices at low Reynolds numbers and the significance of these vortices in terms of their impact on fuel salt velocity and temperatures.

Figure 1.1: Diagram of MSR primary and secondary loops (reproduced from [2]).
Our focus is on the Molten Salt Reactor Experiment (MSRE) [3] (Figures 1.2 and 1.3), a graphite-moderated MSR prototype that is the basis for many modern MSR designs. In this reactor, the molten fuel salt flowed through channels inside a matrix of interconnected graphite prisms called graphite stringers (Section 4.1). We simulated the upward flow of fuel salt around one such stringer along four half-channels that drain into a small part of the upper plenum. We improved upon MSRE simulations found in literature by incorporating the pyramid-tip of the stringer into our mesh. To assess the importance of this commonly neglected feature, we simulated a variety of stringer-tip configurations and assessed their impact on heat transfer using LES with conjugate heat transfer. To our knowledge, this is the first application of LES to the MSRE and the first study focused on analysing the effects of the stringer-tip dimensions on the flow in the MSRE. We hope that these results will inform the design and simulations of future MSRs.

Figure 1.2: Photograph of the MSRE core vessel (reproduced from [3]).
To understand the relevance of this analysis for the nuclear power industry and energy systems at large, further context is required. Global warming caused by greenhouse gas emissions is an urgent planetary threat that will cause
long-lasting and potentially irreversible damage to natural ecosystems. This is due to a predicted rise in average global temperatures and sea levels, and changes to the climate and precipitation patterns [5]. This will likely disrupt our society by adversely affecting agricultural yields, reducing freshwater availability and quality, and increasing the frequency of extreme weather events [6]. Hence, rapidly transitioning to low-carbon energy has become a global priority. Within the electricity supply sector, renewable energy from solar and wind offers significantly reduced carbon emissions compared to fossil fuels, but suffers from the problem of intermittency, requiring energy storage technologies or peaking natural gas power plants for grid stability. Unlike pumped hydropower, batteries are the only commercial low-carbon storage solution that can be deployed without geographic constraints. However, the manufacture of batteries itself creates significant CO₂ emissions [7, 8] and relies on metals that are limited in supply [9, 10]. Carbon Capture and Sequestration (CCS) technologies have yet to be commercialised [11], and they are more polluting than nuclear power when life-cycle emissions are taken into account (Table 1.1). Hydrogen power results in minimal emissions if hydrogen is produced by electrolysis from renewable energy [12], but while hydrogen fuel cells and electrolysers are approaching commercialisation, the development of a supply and distribution network for hydrogen power will likely take years [13].

Table 1.1: Emission coefficient comparison of electricity supply technologies [14].

<table>
<thead>
<tr>
<th>Technology</th>
<th>Lifecycle emissions (g CO₂-eq/kWh)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nuclear</td>
<td>3.7/12/110</td>
</tr>
<tr>
<td>Solar PV (utility)</td>
<td>18/48/180</td>
</tr>
<tr>
<td>Wind (onshore)</td>
<td>7/11/56</td>
</tr>
<tr>
<td>Wind (offshore)</td>
<td>8/12/35</td>
</tr>
<tr>
<td>Gas</td>
<td>410/490/650</td>
</tr>
<tr>
<td>Coal</td>
<td>740/820/910</td>
</tr>
<tr>
<td>CCS Coal (oxyfuel)</td>
<td>100/160/200</td>
</tr>
<tr>
<td>CCS Coal (pulverised coal)</td>
<td>190/220/250</td>
</tr>
<tr>
<td>CCS Coal (integrated gasification combined cycle)</td>
<td>170/200/230</td>
</tr>
<tr>
<td>CCS Coal (combined cycle)</td>
<td>94/170/340</td>
</tr>
</tbody>
</table>

Because of the need for immediate decarbonisation, nuclear power is the only available source of low-carbon baseload power. If it is not decommissioned prematurely, a reactor’s lifecycle emissions per unit electricity produced can be significantly lower than a renewable energy-source’s, especially if the lifecycle emissions of battery backup or the emissions from peaking natural gas plants are also taken into account (Table 1.1). Modern light water reactors have limited load-following capabilities as well [15, 16], making them compatible with a renewable energy-dominant grid. Due to these advantages offered by nuclear power, interest has renewed in developing advanced reactors that are safe, cost-effective, and can be deployed in the near future (Figure 1.4).
One such design is a liquid-fueled channel-type MSR (henceforth referred to as an MSR). These reactors offer several advantages over conventional light water reactors [17, 1]:

- The reactors offer increased safety due to operating pressures close to atmospheric pressure.

- MSRs have passive safety due to a strong negative reactivity coefficient and freeze plugs that allow the fuel salt to drain into subcritical tanks in the event of the core overheating.

- The reduced operating pressures translate into smaller containment vessels compared to light water reactors. This could reduce construction cost and time.

- The high heat capacity of molten salts also makes the primary loop more compact.

- Continuous reprocessing of fuel salt allows management of reactivity without relying on control rods alone.

- Continuous removal of $^{135}\text{Xe}$ using a helium sparging system minimizes dead time [18] after reactor shutdown or power decrease.

- Utilisation of thorium using the $^{232}\text{Th}\rightarrow^{233}\text{U}$ cycle is possible with MSRs. This is an attractive prospect since thorium is more abundant than uranium and produces less transuranic waste than a conventional once-through cycle.

- MSRs can be operated as breeders, converters, or burners [18] that utilise transuranic waste from other reactors.
Currently, multiple MSR designs are under development across the globe. Terrestrial Energy have developed the Integral Molten Salt Reactor [19], a small modular MSR (Figure 1.5). Based on the MSRE and Denatured Molten Salt Reactor [20], it is moderated by graphite and operates as a once-through "burner". Its core is expected to be replaced every 7 years [21]. This design has cleared the Canadian Nuclear Safety Commission's Phase 1 licensing review [22], and the company hopes to build a prototype before 2030.

![Figure 1.5: Terrestrial Energy’s Integral Molten Salt Reactor (reproduced from [21]).](image)

China is constructing an experimental prototype called the Thorium-based Molten Salt Reactor-Liquid Fuelled (TMSR-LF1) (Figure 1.6) [23]. Similar to the MSRE, it is a thermal reactor that is moderated by graphite. Salt flows upwards through the graphite in the core into a plenum, finally exiting the core through an outlet at the top. Terrapower and the Southern Company are developing the Molten Chloride Fast Reactor (Figure 1.7), which promises high efficiency, passive safety, proliferation resistance, and integration with industrial applications [24]. They aim to initiate testing at an experimental test facility in 2021 and complete licensing of a test reactor targeted for operation in the late 2020s [25]. Other recent MSR designs include the reactor from the now-defunct Transatomic
Power [26], Flibe Energy’s Liquid Fluoride Thorium Reactor [27], the Indian Molten Salt Breeder Reactor [28], and Seaborg’s Compact Molten Salt Reactor [29].

Figure 1.6: A diagram of the Chinese TMSR-LF1 prototype reactor, a channel-type liquid-fuelled MSR (reproduced from [23]).

Figure 1.7: A diagram of Molten Chloride Fast Reactor (reproduced from [24]).

However, before these designs are realised, their licensing pathway must be clarified. Brown et al. [30] list multiple reactor physics phenomena that must be investigated for any MSR before its safety can be guaranteed.
They name the study of flow regimes, mixing, and heat transfer as important thermal-hydraulic aspects to be examined. We consider the MSRE to be a prime candidate for such thermal-hydraulic analyses as it serves as the inspiration for many of the aforementioned MSR designs. Results from its study can be extrapolated to similar MSRs and can help inform the thermal-hydraulic studies of future MSRs. Hence, it is necessary to evaluate the thermal hydraulics of the MSRE to assess the safety of MSRE-type reactor prototypes and to verify and validate modern CFD solvers for MSR simulations.

The MSRE, operated by the Oak Ridge National Laboratory (ORNL) from 1964-69, is a historic milestone in the development of MSRs. In addition to demonstrating the viability and the potential of MSRs, it serves as an important, and often exclusive, source of experimental data. The reactor was the first to use $^{233}$U as fuel, demonstrating the viability of a thorium fuelled reactor. It was a graphite-moderated thermal reactor in which fuel salt flowed upward through channels in the graphite matrix. The matrix was composed of graphite bars called stringers. The flow in the channels was laminar. However, the core had lower and upper plena where flow separation occurred, which could have resulted in recirculation vortices. The original MSRE reports [3, 4] do not mention their existence. However turbulent behaviour has been reported in the plena of light water [31] and sodium-cooled [32] reactors. During the course of our work, Podila et al. [33] published a RANS simulation of the MSRE core that exhibits these recirculation or “dead” zones in the upper plenum (Figure 1.8).

In the upper plenum, the pyramid tip of the MSRE graphite stringers can mitigate the vortices formed by the salt jets exiting the channels. However, as meshing the tip is a non-trivial task, researchers often approximate the shape of the MSRE stringer as a flat-topped bar (Figure 1.8). Furthermore, computational limitations, coupled with the low Reynolds number of 1000 in an MSRE channel, have often motivated the use of low- to medium-fidelity turbulence models in CFD simulations of the MSRE. We improved upon these analyses by using LES for a more accurate turbulence model and by incorporating the pyramid tip of the graphite stringer. We also assessed the impact of the stringer shape by simulating four configurations of the pyramid tip. In doing so we investigated the impact of this often neglected part of the MSRE core on the flow and temperature in the upper plenum.

We simulated molten salt flow within an MSRE channel using Nek5000 [34], a Spectral Element Method (SEM)-based CFD solver. We discuss the theoretical background necessary to understand the simulations and relevant parameters in Chapter 2. Chapter 3 provides a literature review of the current state of CFD analyses of MSRs and the motivation for our work. Thereafter, we overview the MSRE reactor design and important simulation parameters in Chapter 4. Chapter 5 presents the results and a brief discussion, followed by a summary of the findings and recommendations for future work in Chapter 6.
Figure 1.8: RANS simulation of the MSRE performed by Podila et al. (reproduced from [33]). Geometry-induced turbulence is visible in both the lower and the upper plenum. Salt recirculation zones are seen above some graphite stringers in the upper plenum. Note that the stringers have a flat top.
Chapter 2

Background

In a molten salt reactor, the salt must remain in the liquid phase during safe operation. Therefore, the salt velocity and temperature in Molten Salt Reactors (MSRs) can be obtained from the Navier-Stokes equations for incompressible flow [35]:

\[ \nabla \cdot \vec{v} = 0 \quad (2.1) \]
\[ \frac{\rho \vec{D}}{\rho \frac{D}{D\tilde{t}}} = -\nabla \tilde{p} + \nabla \cdot \tau + \rho \tilde{f} \quad (2.2) \]
\[ \rho C_p \frac{\tilde{D}T}{\frac{D}{D\tilde{t}}} = \nabla \cdot (k \nabla T) + \tilde{q}''' \quad (2.3) \]

where

\[ \vec{v} = \text{physical velocity [ms}^{-1}] \quad (2.4) \]
\[ \rho = \text{fluid density [kg m}^{-3}] \quad (2.5) \]
\[ \tilde{t} = \text{physical time [s]} \quad (2.6) \]
\[ \frac{\tilde{D}}{\tilde{D}t} = \frac{\partial}{\partial \tilde{t}} + \vec{v} \cdot \nabla = \text{material derivative} \quad (2.7) \]
\[ \vec{x} = \text{physical position used in the } \vec{\nabla} \text{ operator[m]} \quad (2.8) \]
\[ \tilde{p} = \text{pressure [Pa]} \quad (2.9) \]
\[ \tau = \text{stress tensor [Nm}^{-2}] \quad (2.10) \]
\[ \tilde{f} = \text{acceleration from body force [ms}^{-2}] \quad (2.11) \]
\[ T = \text{physical temperature [K]} \quad (2.12) \]
\[ \tilde{q}''' = \text{volumetric heat source [Wm}^{-3}] \quad (2.13) \]
\[ C_p = \text{fluid's isobaric specific heat [Jkg}^{-1}K^{-1}] \quad (2.14) \]
\[ k = \text{fluid's thermal conductivity [Wm}^{-1}K^{-1}]. \quad (2.15) \]
We can simplify the momentum equation (Equation 2.2) by assuming constant viscosity and conductivity, and by using the following constitutive relation [36]

\[ \mathbf{\tau} = \mu (\nabla \mathbf{\tilde{v}} + (\nabla \mathbf{\tilde{v}})^T) \] (2.16)

where

\[ \mu = \text{fluid viscosity [Pa}\cdot\text{s].} \] (2.17)

Additionally [36]

\[ \nabla \cdot \mathbf{\tau} = \mu (\nabla^2 \mathbf{\tilde{v}} + \nabla(\nabla \cdot \mathbf{\tilde{v}})) = \mu \nabla^2 \mathbf{\tilde{v}} \] (2.19)

Substituting this into Equation 2.2, we obtain

\[ \rho \frac{D\mathbf{\tilde{v}}}{Dt} = -\nabla \mathbf{\tilde{p}} + \mu \nabla^2 \mathbf{\tilde{v}} + \rho \mathbf{\tilde{f}} \] (2.20)

Using scaling factors for velocity, time, position, and temperature (see Equations 2.24-2.26, 2.31) the Navier-Stokes equations can be written in their non-dimensionalised form [37]

\[ \nabla \cdot \mathbf{v} = 0 \] (2.21)

\[ \frac{D\mathbf{v}}{Dt} = -\nabla p + \frac{1}{Re} \nabla^2 \mathbf{v} + \mathbf{f} \] (2.22)

\[ \frac{D\theta}{Dt} = -\frac{1}{Pe} \nabla^2 \theta + q''' \] (2.23)

where

\[ v = \frac{\mathbf{\tilde{v}}}{U} = \text{non-dimensionalised velocity [-]} \] (2.24)

\[ x = \frac{x}{L_c} = \text{non-dimensionalised position [-]} \] (2.25)

\[ t = \frac{t}{L_c/U} = \text{non-dimensionalised time [-]} \] (2.26)

\[ \frac{D}{Dt} = \frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla = \text{non-dimensionalised material derivative} \] (2.27)

\[ p = \frac{\mathbf{\tilde{p}}}{\rho U^2} = \text{non-dimensionalised pressure [-]} \] (2.28)
\[ f = \frac{\bar{f} L_c}{U^2} = \text{non-dimensionalised body force} \ [\] \quad (2.29) \]

\[ Re = \frac{\rho U L_c}{\mu} = \text{the Reynolds number} \ [-] \quad (2.30) \]

\[ \theta = \frac{T - T_0}{\Delta T} = \text{non-dimensionalised temperature} \ [-] \quad (2.31) \]

\[ T_0 = \text{reference temperature} \ [K] \quad (2.32) \]

\[ \Delta T = \text{reference temperature difference} \ [K] \quad (2.33) \]

\[ q'''' = \frac{L_c}{\rho C_P U \Delta T} \tilde{q}'''' = \text{non-dimensionalised source term} \ [-] \quad (2.34) \]

\[ Pe = \frac{L_c U}{\rho C_P} = \text{the Peclet number} \ [-] \quad (2.35) \]

\[ L_c = \text{characteristic length} \ [m] \quad (2.36) \]

\[ U = \text{mean velocity} \ [ms^{-1}] \quad (2.37) \]

However, these equations become highly non-linear with increasing Reynolds number (Re). As a consequence, the flow is time-dependent, three-dimensional in character, random, and highly dependent on the flow history and geometry. Therefore, a closed-form analytic solution of the Navier-Stokes equations cannot be obtained for most 3D engineering applications. A numerical approach is necessary to arrive at a solution. Furthermore, the difference between the length scales associated with the largest and smallest eddies widens rapidly with increasing Re [35]. Capturing the behaviour of these smaller eddies in our numerical solution is essential because as the turbulent kinetic energy cascades from larger to smaller eddies, much of the dissipation of this kinetic energy occurs in the smaller eddies. Therefore, it is necessary to discretise the domain of interest with an appropriate grid size to resolve the smallest scales of turbulence and to capture their dissipative physics.

This chapter discusses the theoretical basis for the methods used in the thesis. Large Eddy Simulation (LES), our chosen turbulence model for simplifying the Navier-Stokes equations, is discussed briefly. The discussion of filters develops the background necessary to understand the filter settings in Nek5000, discussed in Chapter 4. The Spectral Element Method (SEM) is also introduced as the discretisation method of choice. We explain why Nek5000 uses spectral elements, what are their advantages over low-order finite elements, and why SEM requires hexahedral meshes. The discussion of spectral elements also explains key simulation parameters in Chapter 4.

## 2.1 Large Eddy Simulation

Direct Numerical Simulations (DNS) [38] solve the Navier-Stokes equations by resolving all scales of motion on fine spatial grids on the order of the Kolmogorov length scale, which is associated with the smallest eddies in turbulent
flow [35] and is given by:

$$\eta = \left( \frac{\nu^3}{\epsilon} \right)^{1/4}$$  \hspace{1cm} (2.38)

where

$$\eta = \text{Kolmogorov length scale} \ [m]$$  \hspace{1cm} (2.39)

$$\nu = \text{kinematic viscosity} \ [m^2 \text{s}^{-1}]$$  \hspace{1cm} (2.40)

$$\epsilon = \text{average rate of dissipation of turbulent kinetic energy per unit mass} \ [m^2 \text{s}^{-3}]$$  \hspace{1cm} (2.41)

The solutions generated are extremely detailed and can serve as surrogates for experimental data used for verifying other Computational Fluid Dynamics (CFD) solvers or models. This level of detail comes with a high price – the computational cost of direct numerical simulation scales with Re^{3.5} [35], making this approach intractable for moderate to high Re flows. Most DNS computational operations focus mainly on the smallest scales of dissipative flow, but most of the energy, anisotropy, and flow characteristics are contained in the larger eddies. Large Eddy Simulation (LES) makes a compromise that lowers computational costs significantly, yet represents turbulent flow more accurately than Reynolds-Averaged Navier Stokes (RANS) models [39]. In LES, the large scale eddies are resolved and simulated directly. The smaller scale eddies, which have uniform properties relative to large scale eddies over a given domain, are represented by simpler models such as a sub-grid scale model [40] or a filter [35] which capture the dissipative behaviour of these eddies. This way, most of the computational effort focuses on large scale turbulent flow, which describes flow properties of interest in sufficient detail for most engineering applications [35]. We also need fewer grid points to resolve the larger scales of turbulence, which results in significant computational savings.

The main components of an LES model are the filter, the formulation of filtered equations, and the closure model.

**The Filter:** In LES, the velocity \( \mathbf{U}(x, t) \) is decomposed into a filtered, random component \( \mathbf{U}'(x, t) \) representing large eddies and a non-zero residual or sub-grid scale component \( \mathbf{u}'(x, t) \) that represents smaller scale motions, that is

\[
\mathbf{U}(x, t) = \mathbf{U}(x, t) + \mathbf{u}'(x, t) \tag{2.42}
\]

\[
\mathbf{U}(x, t) = \text{unfiltered velocity} \ [ms^{-1}] \tag{2.43}
\]
\( \bar{u}(x, t) = \) filtered velocity \([m s^{-1}]\) \hspace{1cm} (2.44)

\( u'(x, t) = \) residual or sub-grid scale velocity \([m s^{-1}]\) \hspace{1cm} (2.45)

This is accomplished with a low-pass filtering operation with a *filter width*, \( \Delta \), that is ideally slightly smaller than the size of the smallest eddies. The grid spacing required for LES is proportional to \( \Delta \). A more mathematically rigorous definition of \( \Delta \) uses the length scale \( l_{el} \) [35], given by

\[
l_{el} = \frac{1}{6} \frac{1}{< u'^2 >} \int_0^\infty R(r) dr \tag{2.46}
\]

where

\[ u(x) = U(x) - < U(x) >= \text{fluctuating component of turbulent velocity \([m s^{-1}]\)} \tag{2.47} \]

\[ R(r) = < u(x+r)u(x) >= \text{the autocovariance function at } r \ [m^2 s^{-2}] \tag{2.48} \]

\[ U(x) = \text{the velocity at x \([m s^{-1}]\)} \tag{2.49} \]

In 3D, using \( \Delta \approx l_{el} \) usually resolves about 80% of the energy spectrum [35].

Since the size of the smallest eddies is significantly larger than the Kolmogorov length scale, this filtering operation allows \( U(x, t) \) to be resolved on a much coarser grid than one required to resolve the velocity field in direct numerical simulation. In 3D, an appropriately chosen filter width can resolve 80% of the energy spectrum of the flow on a much coarser grid than the one used for DNS [35].

**Formulation:** Equations for the filtered velocity are derived directly from the Navier-Stokes equations. The momentum equation contains the residual stress or sub-grid scale stress tensor that stems from the sub-grid scale component \( u' \). An example of filtered equations is presented in Appendix A.

**Closure:** Closure is obtained by approximating the aforementioned sub-grid scale stress with simplified models such as the Smagorinsky model [40]. Since such a model provides numerical dissipation to stabilise the simulation, LES can also be performed without an explicit sub-grid scale model, and can instead use filters to provide the required dissipation.

These components are universal to all LES models. However, in practice, the LES methodology must be adapted to the application at hand. An especially challenging problem emerges when modelling near-wall flows. The viscous wall region is important as production and dissipation of kinetic energy and Reynolds stress terms peak within 20
viscous length scales of the wall. However, the viscous-length scale varies with the Reynolds number as:

$$\frac{\delta_v}{\delta} \sim Re^{-0.88}$$ (2.50)

where

$$\delta_v = \text{viscous length scale [m]}$$ (2.51)

$$\delta = \text{channel half-height [m]}.$$ (2.52)

To resolve near-wall eddies, the grid-spacing, $\Delta x$, and the filter width, $\Delta$, must be on the order of $\delta_v$ [35, 38, 41]. Accordingly, the number of nodes increases as $Re^{1.76}$ near the wall [42]. This makes simulating near-wall flows computationally expensive, even with LES. Approaches to dealing with this challenge lead to three broad categories of LES – LES with near-wall resolution, LES with near-wall modelling, and very large eddy simulation.

**LES with near-wall resolution** In this approach, the filter and the grid are fine enough to resolve the flow everywhere, including near the wall. This is computationally expensive for high Re flows.

**LES with near-wall modelling** The grid and filter are chosen to resolve the flow far from the wall, but in the near-wall region, modelling similar to sub-grid scale models is used and direct resolution as in DNS is avoided. This makes large eddy simulation more tractable for near-wall flows.

**Very large eddy simulation** The filter and the grid are coarse and do not resolve most energy-containing motions. It can be inexpensive computationally, but its accuracy depends on the sub-grid scale model employed.

### 2.1.1 Filtering

This section introduces the mathematical operations involved in filtering and the background necessary to understand the filter used in our Nek5000 simulations (see Chapter 4.2). Numerically, filters serve a function similar to sub-grid scale models - they provide artificial viscosity that stabilizes LES. This is why Nek5000, our chosen CFD solver, has no explicit sub-grid scale model like the classical Smagorinsky [43] or dynamic Smagorinsky model [44], as the filter provides the dissipation instead.

A typical filtering operation is defined using a *filter function* $G(r,x)$ acting at a point $r$ on the velocity field. Mathematically, it is given by [45]

$$\overline{U}(x, t) = \int G(r,x) U(x - r, t) \, dr$$ (2.53)
where \( r \) varies over the entire flow domain and the filter function is normalised, i.e.

\[
\int G(r, x) dr = 1 \tag{2.54}
\]

The action of a filter on the velocity field can be understood in terms of its effect in physical space, or in terms of the action of its Fourier transform \( \hat{G}(K) \) on the velocity field's Fourier transform in wavenumber space. The Fourier transforms of filter functions are called transfer functions, given by

\[
\hat{G}(K) = \int_{-\infty}^{\infty} e^{-iKr} G(r) dr \tag{2.55}
\]

For instance, a box filter, which looks like a box in physical space, is given by

\[
G(r) = \frac{1}{\Delta} H\left(\frac{1}{2}\Delta - |r|\right) \tag{2.56}
\]

\[
\hat{G}(K) = \frac{\sin(\frac{1}{2}\sin(K\Delta))}{\frac{1}{2}\sin(K\Delta)} \tag{2.57}
\]

where

\[
H(x) = \frac{d}{dx} \max\{|x, 0| = \text{the Heaviside step function.} \tag{2.58}
\]

As Equation 2.56 indicates, the box filter is localised in the physical space and it averages velocity in the physical space around \( x \pm \frac{1}{2}\Delta \). However, its action in wavenumber space is not localised. The spectral filter, on the other hand, given by

\[
G(r) = \frac{\sin(\pi r / \Delta)}{\pi r} \tag{2.59}
\]

\[
\hat{G}(K) = H(K_c - |K|) \tag{2.60}
\]

where

\[
K_c = \frac{\pi}{\Delta} = \text{cutoff wavenumber}
\]

is localised in wavenumber space in that it annihilates all Fourier modes with wavenumber greater than the cut-off wavenumber \( K_c \), but it is diffused in physical space. This makes it more suitable than the box filter for annihilating
high wavenumber modes, which contain most of the discretisation error [35]. The Gaussian filter, given by

\[ G(r) = \left( \frac{6}{\pi \Delta^2} \right)^{1/2} \exp \left( -\frac{6r^2}{\Delta^2} \right) \]  

(2.61)

\[ \hat{G}(K) = \exp \left( -\frac{K^2 \Delta^2}{24} \right) \] 

(2.62)

is localised in neither physical nor wavenumber space, but it is fairly compact in both. While spectral cutoff filters are straightforward to implement and can aggressively dampen high-error modes, they are known to pollute low wavenumbers across multiple elements in a domain [46]. Therefore, Gaussian-like filters are often employed to mitigate this effect.

The choice of filter also affects the grid spacing required to resolve \( \Pi(x) \). For example, for a sharp spectral filter, Pope [35] demonstrates that for \( x \in [0, L] \), the grid spacing required is

\[ h = \frac{\pi}{K_c} \] 

(2.63)

Furthermore, the computational cost of LES scales with \((h/\Delta)^{-4}\) for a given \( \Delta \). Doubling the resolution by halving \( h \) increases the computational costs by a factor of 16. Therefore, the use of appropriate filters and grid resolution is vital to ensure that LES costs remain tractable.

### 2.2 Spectral Element Method

The Spectral Element Method (SEM) is a type of numerical discretisation method based on the Galerkin method. Introduced in 1984 by Patera [47], SEMs are a subset of a class of Finite Element Methods (FEMs) called p-type finite elements (see Section 2.2.2). They are similar to p-FEM in that they use high-degree polynomials on a coarse mesh to obtain high accuracy with relatively few degrees-of-freedom [37]. However, they are also similar to h-type finite elements in that they use Lagrangian interpolation and basis functions with local support [37]. However, spectral element solvers outperform finite element solvers in accuracy and speed due to the use of Gauss-Lobatto-Legendre quadrature and matrix-free tensor product forms [37]. This speed and accuracy is especially useful for simulating highly random and dispersive phenomena such as turbulence, in which the energy cascade from large to small eddies must be modelled accurately over long distances with minimal discretisation-based numerical dispersion. High-order methods like SEM are also able to resolve boundary layers better than low-order methods like h-FEM [48, 49]. For this reason, they are an ideal choice for implementing Direct Numerical Simulations (DNS) and Large Eddy Simulation (LES).

As our work utilises Nek5000 (see Section 4.2), a spectral element Computational Fluid Dynamics (CFD) solver,
the following section introduces key ideas of SEM, and justifies our choice of using a spectral element solver over a finite element solver.

2.2.1 Method of Weighted-Residuals and the Weak Form

All finite element methods arise from the method of weighted residuals, in which the integral of the residual of a differential equation with respect to some weight functions is set to zero over a whole domain \([50, 51]\). In other words, the residual is made orthogonal to the weight functions. These weight functions are used as a linear basis to approximate the solution to the differential equation. Since the residual is orthogonal to the basis functions, this leads to minimal error with respect to those weight functions as none of the residual components lie along the weight functions in the basis. In particular, the Galerkin formulation \([51]\) will be used, in which the weight functions are orthogonal polynomials. Due to integration-by-parts during this process, the method of weighted residuals reduces the differential equation to a weak form (see Equation 2.73) for which a numerical approximation can be obtained from a vector subspace. Discretising this weak form yields a linear system which provides a numerical solution to the differential equation.

As an illustrative example, consider the Poisson problem with homogeneous Dirichlet boundary conditions on the domain \(x \in [a, b]\), that is

\[
-\nabla^2 \tilde{u} = f(x) \quad (2.64)
\]

\[
\tilde{u}(a) = \tilde{u}(b) = 0 \quad (2.65)
\]

where

\[
\tilde{u} = \text{analytical solution} \quad (2.66)
\]

\[
f(x) = \text{arbitrary RHS of Poisson equation.} \quad (2.67)
\]

The weighted residual formulation \([51]\) is as follows: we seek a trial function, \(u\), our approximate solution, in the finite, N-dimensional trial space \(X_0^N \subset H_0^1\), \(u \in X_0^N\) such that the residual \(r\):

\[
r = -\nabla^2 u - f(x) \quad (2.68)
\]

is orthogonal to all test functions \(v \in Y_0^N \subset H_0^1\) in the test space \(Y_0^N\), where \(H_0^1\) is the Sobolev space \([37]\) for our domain whose vectors satisfy the homogeneous Dirichlet boundary condition. The subscripts 0 indicate that all the
basis functions in this subspace satisfy the homogeneous boundary condition. The orthogonality of the residual to
the test functions implies that the $L^2$ norm \(37\) of the residual with all test functions $v$ in the test space is zero. In
the Galerkin method for the Poisson equation, the test and the trial spaces are the same, i.e. $X^N_0 = Y^N_0$. Therefore,
the formulation is

\[
\int_a^b v r \, dx = \int_a^b v (\nabla^2 u + f) \, dx = 0; \ \forall \ v \in X^N_0 \\
\Rightarrow \int_a^b -v \nabla^2 u \, dx = \int_a^b v f \, dx. \quad (2.69)
\]

It appears that $u$ must be twice-differentiable, which would severely restrict the solution space and omit many
discontinuous functions which may be necessary to approximate the analytical solution. However, using integration
by parts, we obtain

\[
\int_a^b -v \nabla^2 u \, dx = \int_a^b \nabla v \nabla u \, dx - v \nabla u^b_a \\
= \int_a^b \nabla v \nabla u \, dx. \quad (2.70)
\]

where the boundary terms vanish due to homogeneous Dirichlet boundary conditions. Therefore, the weak form of
the Poisson equation is

\[
\int_a^b \nabla v \nabla u \, dx = \int_a^b v f \, dx. \quad (2.71)
\]

The integral on the left hand side is known as the energy inner product or "a" inner product

\[
a(v, u) = \int_a^b \nabla v \nabla u \, dx. \quad (2.74)
\]

The inner product is symmetric. If we assume that there exists a unique solution in our chosen Sobolev space, the
Lax-Milgram theorem \(37\) also requires that this inner product be positive-definite. Depending on the problem,
these integrals may be evaluated directly, especially for low-order finite elements. But for high-order methods like
SEM, and for certain forms of the function $f$, numerical integration through quadratures \(52\) is recommended.

As $v \in X^N_0$, and in the Galerkin method, $X^N_0$ is a set of orthogonal polynomials from the subspace

\[
X^N_0 = \{ \phi_1, \ldots, \phi_N \} \quad (2.75)
\]
where

\[ \phi_i = \text{orthogonal basis polynomials.} \] (2.76)

Therefore the LHS of the weak form can be written as

\[ a_{ij} = \int \nabla \phi_i \nabla \phi_j \, dx \] (2.77)

where

\[ a_{ij} = \text{elements of the stiffness matrix } A \] (2.78)

and the RHS can be expressed as:

\[ b_i = \int_a^b \phi_i f(x) \, dx . \] (2.79)

However, the exact integral above is never evaluated. Instead, \( f(x) \) is interpolated on the test space at \( N \) discrete points using the \( N \) basis functions as:

\[ f(x) = \sum_{j=1}^{N} f(j_i) \phi_j \] (2.80)

Substituting this into the expression for \( b \) (Equation 2.79), we get

\[ b = \sum_{j=0}^{N} f(x_j) \int \phi_i \phi_j \, dx \] (2.81)

\[ b = B \tilde{f} \] (2.82)

where

\[ B = \text{mass matrix, with } b_{ij} = \int \phi_i \phi_j \, dx \] (2.83)

\[ \tilde{f} = f(x_j) = f(x) \text{ at } N \text{ discrete nodes.} \] (2.84)

This procedure yields the discretised version of the Poisson equation as:

\[ Au = B \tilde{f} = b. \] (2.85)

Due to the aforementioned properties of the energy inner product, the matrix \( A \) is symmetric positive-definite.
This property is desirable for many reasons, chief among them that it enables the use of fast iterative methods like conjugate gradients [53]. While we have assumed homogeneous Dirichlet boundary conditions, others, including inhomogeneous boundary conditions can be applied by splitting the solution into homogeneous and inhomogeneous parts, using restriction/prolongation matrices to solve for just the homogeneous solution and superimposing the inhomogeneous part thereafter [37, 53].

2.2.2 Comparison of finite and spectral elements

FEM approximations to solving differential equations involve discretising the domain into a network of smaller elements called a mesh. Then, the differential equation is discretised over each element using the aforementioned Galerkin approach. The choice of test space is limited to polynomials that are highly local to each element - they terminate in the element itself or in the adjacent elements. Common choices include linear and quadratic polynomials, and cubic splines [50]. Typical mesh elements are triangles in 2D and tetrahedrons in 3D [51].

There are two approaches to finite elements - h-type FEM and p-type FEM [37]. In h-FEM, the order of the test functions is fixed, usually to linear or quadratic elements. Accuracy is achieved by holding the order of the test functions constant, and increasing the number of elements in the mesh. In p-type FEM, the approach is the inverse of h-FEM: the number of elements is fixed, and accuracy is achieved by increasing the order of the basis polynomials. Consequently, p-FEM discretisations have coarser elements and a high number of intra-element nodes. As the number of these nodes increases, so does the accuracy of quadratures involved in the Galerkin discretisation. Thus, with increasing order of basis polynomials, the computed stiffness matrix $A$ and hence the numerical solution $u$ get more accurate.

The main drawback of the p-FEM approach is that the computational and storage costs in memory increase rapidly with increasing polynomial order in higher dimensions. This makes polynomial order of p>4 practically infeasible in 3D [37]. Consider a 1D differential equation discretised to form the stiffness matrices $A_x$. The 3D stiffness matrix for the 3D version of the same problem is often formed explicitly in p-FEM codes using tensor products. For a $p = N - 1^{th}$ order p-FEM method, the $N^3 \times N^3$ 3D stiffness matrix is [37]:

$$A = (B_z \otimes B_y \otimes A_x) + (B_z \otimes A_y \otimes B_x) + (A_z \otimes B_y \otimes B_x) \quad (2.86)$$

where

$$B_x, B_y, B_z = \text{mass matrices of the same size as } A_x, A_y, \text{and } A_z \text{ respectively} \quad (2.87)$$

$$\otimes = \text{the Kronecker product, given by} \quad (2.88)$$
Explicit formation of these operators leads to high-bandwidth matrices \[54\] that are full if the mass matrices \(B_i\) (Equation 2.86) are full or at least high-bandwidth if the mass matrices are diagonal (as is the case for SEM). For \(N \times N\) \(A_x, A_y,\) and \(A_z\) matrices, the stiffness matrix \(A\) will have \(N^6\) nonzeros. If the system is solved by a direct method such as an LU factorisation followed by backward solves, the cost will be \(O((N^3)^3)\) for the factorisation and \(O((N^6)^2)\) for the solution \[54\]. If using iterative methods \[53\], each iteration requires matrix-vector multiplications of the type \(Au\) which will cost \(2N^6\) operations per iteration. As we will demonstrate shortly in this section, SEM reduces this work by two orders of magnitude.

Spectral methods were developed in parallel with finite elements using similar weighted residual approaches \[55\]. They involve using a weighted-residual approach to approximate the solution to a partial differential equation with a truncated sum of basis functions expressed as a discrete Fourier transform, such as

\[
\psi_n = \text{trial functions. (2.92)}
\]

This Fourier approximation is substituted into the differential equation to solve for the expansion coefficients.

The main difference between spectral methods and finite elements is the choice of the test and trial space. Spectral spaces choose high-order, global, infinitely differentiable functions, whereas finite elements choose highly local functions that are not infinitely differentiable \[56\]. These traits make spectral methods extremely accurate as very high order polynomials can be used. However, unlike finite-elements, they are challenging to implement for complex geometries. Spectral methods evolved to use the Galerkin approach with Gaussian quadratures. This improved their speed and accuracy.

However, for higher dimensions, spectral methods also become prohibitively expensive. Forming a 3D discrete Fourier transform also ends up requiring \(O(N^6)\) operations. In order to improve the performance of spectral methods, Orszag \[57\] demonstrated that a three-dimensional Fourier transform can be represented as three one-dimensional Fourier transforms using tensor contractions. This insight can be applied to the action of a 3D operator.
on an operand, which can be expressed as the action of three one-dimensional operands without ever explicitly forming the 3D operator matrix, provided the 1D operators are distinct and separable along three axes. Separating these operators and reducing the tensor product form to matrix-matrix products also lowers the cost of calculating the action of a 3D operator. For these reasons, this approach is known as fast matrix-free tensor product evaluation. This key feature of spectral methods makes the use of high-order polynomials as test and trial functions tractable, resulting in superior accuracy compared to standard p-FEM methods. This is the reason why we are using a spectral element solver.

A modern implementation [37] of this tensor contraction approach is described in Appendix B. On analysing this implementation, two important details emerge. First, in 2D, the original tensor product-based operation evaluation (Equation B.4) would require $2N^4$ operations, whereas the operator-free matrix-vector products need only $4N^3$ operations. Similarly, in the 3D case (Equation B.13), tensor contractions reduce $2N^6$ operations to $3 \times 4N^3$ operations. Comparing the 2D and 3D cases, it is apparent that as dimensions increase, these tensor-contractions become more and more efficient. As turbulence is a 3D phenomenon, this matrix-free approach can result in significant computational savings. Second, the separability of operators along each dimension is crucial for the success of spectral methods. This is possible in square (2D) and hexahedral (3D) elements, where nodes are placed along three distinct orthogonal axes coincident with the sides of a square or cube, but not in triangular (2D) or tetrahedral (3D) elements, as their sides are not orthogonal. This is why Nek5000 requires hexahedral meshes in 3D.

Orszag [57] also pointed out that spectral test functions had to be infinitely differentiable and had to satisfy unrealistic boundary conditions (such as the periodic boundary conditions) in order for spectral expansions of functions in said test space to converge rapidly. He demonstrated that spectral methods converge rapidly if orthogonal polynomials (e.g.: Chebyshev or Legendre) are used. Then, the spectral convergence depends only on the smoothness of the test function. This also mitigates the Gibbs phenomenon.

Patera [47] based his work on the similarity between the Galerkin formulation of spectral methods and the quadrature-based form of p-FEM, and formulated SEM. It is a subset of p-FEM methods in which high-order orthogonal polynomials are used as basis functions on a coarse mesh, along with Gauss-Lobatto-Legendre quadrature [51] and matrix-free operators. While Chebyshev polynomials were used initially, most SEM methods now use Legendre polynomials as the weighing factors for quadrature are simpler for the latter, leading to a more straightforward implementation [37]. The fast matrix-free tensor product evaluation is implemented in every element to improve computational speed. The use of Gauss-Lobatto-Legendre quadrature improves operator conditioning, suppression of the Runge phenomenon [54], ease of implementing boundary conditions, and high accuracy – an N-point quadrature is exact for all integrands that are in the space of polynomials of order 2N-1.

Formulated as a hybrid spectral-finite element approach, SEM provides the advantages of both p-FEM and
spectral methods. Mesh-based finite-element discretisation enables accurate representation of complex geometries and a wide range of boundary conditions, while tensor contractions and Gauss-Lobatto-Legendre quadrature from a spectral approach ensures high-accuracy with low computational and memory costs.

### 2.3 Spectral element solution of incompressible Navier-Stokes

While we have discussed the advantages of spectral elements over the finite elements, it is also necessary to consider a brief overview of the spectral elements solution to incompressible Navier-Stokes equations, in order to understand how the pressure and velocity solvers in Nek5000 work and our choice of input parameters in our simulations (see Section 4.3.2). The weak formulation of Navier-Stokes equations (Equation 2.21) is as follows: let the trial functions for the velocity and pressure be \((u, p) \in X_b^N \times Y_0^N\). The test functions for orthogonalising the residuals are \((v, q) \in X_b^N \times Y_0^N\).

\[
\frac{d}{dt} \int v u d x + \frac{1}{Re} \int \nabla v \nabla u d x = - \int \nabla v p d x - \int v u \cdot \nabla u d x + \int v f d x \tag{2.93}
\]

\[
(q, \nabla \cdot u) = 0. \tag{2.94}
\]

The dimensions of the pressure space will be discussed towards the end of this section. The advection operator is given by:

\[
c(v, u) = \int v u \cdot \nabla u d x = - \int u u \cdot \nabla v d x = -c(u, v) \tag{2.95}
\]

where we have used integration by parts, as previously, and have exploited assumed homogeneous boundary conditions and the divergence-free property of incompressible flow [55]. Note that the advection operator is skew-symmetric, and has purely imaginary eigenvalues, which makes it easy to stabilise in time stepping schemes by simply reducing the time step size [37].

Since, on each element, \(v\) is in an \(N\)-dimensional subspace, the advection operator \((- \int v u \cdot \nabla u d x)\) lies in the \(3N\)-dimensional subspace. Recall that an \(N\)-point Gauss-Lobatto Legendre quadrature rule is exact for integrands of degree \(2N-1\) or less. So, while an \(N\)-point Gauss-Lobatto-Legendre quadrature may suffice for other Navier-Stokes terms, it will be inaccurate for the \(3N\)-dimensional advection operator due to subsampling, or aliasing. Any degree of imprecision in the advection operator greatly destabilises time stepping in unsteady Navier-Stokes discretisations, as the inexact advection operator is no longer skew-symmetric, and has imaginary eigenvalues with real components. Since such eigenvalues occur in conjugate pairs, one will invariably lie outside the neutral stability curve [54] of our time stepper[37]. Those eigenmodes will eventually destabilise the solution. Physically, as the advection term term is responsible for generating turbulence, it is vital to obtain an accurate representation of it.
Accordingly, a quadrature of order \((3N + 1)/2\) is required to adequately sample, or *dealias*, the advection operator. This is known as the 3/2 dealiasing rule. In practice, it would be computationally wasteful to integrate anything but the advection operator with this higher order quadrature. Therefore, the advection operator is interpolated to a finer grid, integrated by quadrature, then re-interpolated to the coarse grid on which the other operators are integrated. This also explains our choice of the dealiasing parameter in Nek5000 (Chapter 4).

Note that the diffusion term is being treated implicitly on the LHS, whereas the advection term is treated explicitly on the RHS. Physically, this is due to the fact that diffusion happens on a smaller time scale than advection, so for "faster" phenomena, we use the velocity value from the latest time step available. Numerically, this treatment offers improved stability during time stepping and ensures that the LHS matrix is symmetric and positive-definite. This would not be possible if the advection operator were treated implicitly and incorporated into the LHS, since the advection operator would add its imaginary eigenvalues to the LHS matrix. This symmetry enables the use of fast iterative methods, like conjugate gradients [53].

After obtaining operator matrices and dealiasing the advection operator, we obtain:

\[
B \frac{du}{dt} + vAu - DTp = Cu + Bf 
\]

\[
Du = 0 
\]

where

\[
A = \text{stiffness matrix} 
\]

\[
B = \text{mass matrix} 
\]

\[
C = \text{dealiased advection operator} 
\]

\[
D = \text{derivative operator.} 
\]

Using the Backward Difference/Extrapolation (BDFk/EXTk) time stepping scheme[37], we can approximate the time derivative on the LHS of Equation 2.96 using BDFk as:

\[
B \frac{du}{dt} = \frac{1}{\Delta t} \left( \beta_0 Bu^n + \sum_{j=1}^{k} \beta_j Bu^{n-j} + O(\Delta t^k) \right) 
\]

where

\[
\Delta t = \text{time step size} 
\]
\[ u^n = \text{velocity value at the } n^{th} \text{ time step} \]  
(2.104)

\[ \beta_0, \beta_k = \text{the BDFk/EXTk coefficients} \]  
(2.105)

\[ O(\Delta t^k) = \text{time-discretisation error}. \]  
(2.106)

For the RHS of Equation 2.96, we can use the extrapolation scheme EXTk to obtain

\[ \tilde{b} = Cu + Bf = -\sum_{j=1}^{k} \alpha_j (Cu^{n-j} - Bf^{n-j}) \]  
(2.107)

where

\[ \alpha_j = \text{the } k^{th} \text{ order BDFk/EXTk extrapolation coefficients} \]  
(2.108)

\[ f^n = \text{forcing function at the } n^{th} \text{ time step.} \]  
(2.109)

Substituting these results from Equation 2.102 and 2.107 into the LHS and RHS of Equation 2.96, collecting the \( n^{th} \) time step terms on the LHS, and collecting all previous time step terms on the RHS, we can write

\[ \beta_0 Bu^n + \nu \Delta t Au^n - \Delta t D^T p^n = -\sum_{j=1}^{k} \beta_j Bu^{n-j} - \Delta t \left[ \sum_{j=1}^{k} \alpha_j (Cu^{n-j} - Bf^{n-j}) \right] \]  
(2.110)

Writing the above equation in matrix form along with the divergence-free constraint on the velocity, we obtain

\[ (\beta_0 B + \nu \Delta t A)u^n - \Delta t D^T p^n = b^{n-1} \]  
(2.111)

\[ Du^n = 0 \]  
(2.112)

\[ \Rightarrow \begin{bmatrix} H & -\Delta t D^T \\ -D & 0 \end{bmatrix} \begin{bmatrix} u^n \\ p^n \end{bmatrix} = \begin{bmatrix} b \\ 0 \end{bmatrix} \]  
(2.113)

where

\[ H = \beta_0 B + \nu \Delta t A = \text{the Helmholtz operator} \]  
(2.114)

\[ b = \text{RHS of Equation 2.110.} \]  
(2.115)

Solving for both velocity and pressure at the same time can be computationally expensive [37]. It is preferable to decouple the velocity and pressure equations, then to solve for the pressure followed by the velocity in separate steps. In order to decouple the pressure and velocity equations, we perform block Gaussian elimination [54] on
the LHS matrix. First, we multiply the first equation by the inverse of the Helmholtz operator $H^{-1}$, obtaining an equation with the tentative velocity $u^*$ which is not divergence-free:

$$
\begin{bmatrix}
I & -\Delta t H^{-1} D^T \\
-D & 0
\end{bmatrix}
\begin{bmatrix}
u^n \\
p^n
\end{bmatrix}
= 
\begin{bmatrix}
H^{-1} b \\
0
\end{bmatrix}
= 
\begin{bmatrix}
u^*
\end{bmatrix}
$$

(2.116)

where

$$u^* = H^{-1} b = \text{tentative velocity (not divergence-free)}. \quad (2.117)$$

Next, we multiply the equation in the first row of the above matrix by $-D$, and subtract it from the second row, obtaining:

$$
\begin{bmatrix}
I & -\Delta t H^{-1} D^T \\
0 & \Delta t D H^{-1} D^T
\end{bmatrix}
\begin{bmatrix}
u^n \\
p^n
\end{bmatrix}
= 
\begin{bmatrix}
u^*
\end{bmatrix}
$$

(2.118)

Using these equations, we can solve for the tentative velocity using best-estimates from previous time steps, then the pressure, and finally use the pressure to obtain the correct, divergence-free velocity. This is known as the Uzawa algorithm [58].

The most computationally expensive step is the pressure solve, in which we must use $H^{-1}$ (typically without directly forming the inverse). Many techniques exist to reduce the cost of this step. The Fractional Step Method [59, 60] involves using Taylor series approximations of $H^{-1}$. The Pressure Correction Algorithm [61, 62] is a predictor-corrector type method that uses the pressure gradient from the previous time step to solve the momentum equation. Then, a pressure correction is obtained from a simplified pressure equation similar to the previous equation. The velocity is corrected based on the newly obtained pressure, effectively projecting it into a divergence-free subspace. Nek5000 uses the latter method.

We began with the simplistic assumption that $p \in Y_0^N$. In practice, however, using an $N$-dimensional subspace for both velocity and pressure (known as the $P_N - P_N$ formulation) without any additional modifications when solving incompressible Navier-Stokes equations results in spurious pressure modes [63, 64]. This is because the solution obtained with order-$N$ polynomials for both $u$ and $p$ is not unique [65, 66]. A simple workaround, known as the $P_N - P_{N-2}$ formulation [67], uses staggered spectral elements to find the pressure in $Y_0^{N-2}$. This eliminates these spurious modes by simply going to a smaller subspace where these modes are absent and the solution to the pressure variable is unique [68, 69]. However, Tomboulides et al. [70] have developed methods that make it possible to stabilise the $P_N - P_N$ method [37], making it more accurate for pressure solves since it provides a larger subspace
for pressure trial functions (and consequently, more nodes in each element to resolve the pressure) than $P_N - P_{N-2}$ does. In Nek5000, it is possible to choose either formulation, but we choose $P_N - P_N$ for the advantages mentioned above.
Chapter 3

Literature Review

High fidelity thermal-hydraulics simulations of nuclear reactors that incorporate turbulence are computationally expensive. The high computational cost of these simulations arises largely from the fine spatial resolution required to accurately model turbulent structures, especially near walls and in transitional regions such as plena. The spatial resolution of the mesh, in turn, limits the maximum size of the time step due to the Courant-Friedrichs-Lewy (CFL) condition [37]. The exact numerical formulation of the CFL constraint depends on factors such as whether the time stepping scheme is implicit or explicit, the type of differential equations being solved (parabolic, hyperbolic or elliptic), the spatial discretisation scheme, and the eigenvalues of the operator matrices obtained from the discretisation of the differential equation. For example, consider an unsteady advection problem solved by an explicit finite difference scheme in one dimension. For the imaginary eigenvalues of the skew-symmetric advection operator [37], we have

$$ (\max |\lambda_k|)dt < C_t $$

(3.1)

where

$$ \lambda_k = \text{the } k^{th} \text{ imaginary eigenvalue of the advection operator} $$

(3.2)

$$ dt = \text{time step size} $$

(3.3)

$$ C_t \sim 1 = \text{order-unity constant associated with the timestepper.} $$

(3.4)

For most spatial discretisations, we can relate the maximum-modulus eigenvalue to the local ratio of the advection velocity and the grid spacing [37]:

$$ \max |\lambda_k| \approx C_s |\frac{c}{dx}| $$

(3.5)
where

\[ c = \text{advection velocity} \]  \hspace{1cm} (3.6)

\[ \text{dx} = \text{grid spacing} \]  \hspace{1cm} (3.7)

\[ C_s \sim 1 = \text{order-unity constant dependent on the spatial discretisation (e.g.: in the case of the Spectral Element Method (SEM), on the mesh's polynomial order).} \]  \hspace{1cm} (3.8)

Together, Equations 3.1 and 3.5 lead to the CFL condition:

\[ \frac{c \Delta t}{\Delta x} \leq C_{\text{max}} \]  \hspace{1cm} (3.9)

where

\[ c = \text{advection velocity} \]  \hspace{1cm} (3.10)

\[ \Delta x = \text{smallest spatial grid spacing} \]  \hspace{1cm} (3.11)

\[ \Delta t = \text{largest possible time step size} \]  \hspace{1cm} (3.12)

\[ C_{\text{max}} = \frac{C_t}{C_s} = \text{order-unity constant dependent on the time stepping scheme and spatial discretisation.} \]  \hspace{1cm} (3.13)

The condition restricts the movement of the fluid to no more than one spatial step in one time step. Similar constraints can also be derived from growth factor analysis of time steppers \[54\] and stability curves of time-stepping methods \[37\]. As evident from the equation, a small \( \Delta x \) leads to a small \( \Delta t \), especially for advection-dominated flows. Increasing \( \Delta t \) beyond this limit can introduce numerical instabilities in the solution. Unfortunately, the time scale at which most thermal-hydraulic transients occur is many orders of magnitude larger than the maximum time step size these simulations are restricted to. This leads to long runtimes for high-fidelity Computational Fluid Dynamics (CFD) solvers. In modelling turbulence using LES or DNS, some transients can require wall clock times of the order of years \[71, 35\].

Consequently, CFD simulation costs must be reduced by simplifying simulation approaches. Such simplifications include, in increasing order of complexity: using a prescribed uniform velocity field, 1D Navier-Stokes models with empirical correlations, 2D Navier-Stokes solutions with approximations and empirical correlations, and Reynolds-Averaged Navier Stokes (RANS) turbulence models. Many such methods have been used in multiphysics simulations of Molten Salt Reactor (MSR)s.

Early work by Lecarpentier and Carpentier \[72\] conducted a 1D multiphysics analysis of an Molten Salt Reactor
Experiment (MSRE)-based reactor concept using two-group neutron diffusion, a prescribed uniform velocity field, and simplified thermal-hydraulics based on energy balance. Zhang et al. [73] studied the Molten Salt Advanced Reactor Transmuter (MOSART) reactor using a prescribed uniform velocity field along with Point-Reactor Kinetics Equations in 2009. Yamamoto et al. [74] simulated an MSR concept using 1D Navier-Stokes-based thermal-hydraulics with empirical correlations for heat transfer. Using a similar approach implemented in DYN3D-MSR, Kre pel et al. [75] modelled the MSRE and validated their results against MSRE kinetics and power measurements. Wang et al. [76] performed a 2D coupled neutronic thermal hydraulic analysis of MOSART in the SIMMER-III code, which uses a first order discretisation of Euler equations with a semi-empirical approach to turbulence modelling [77]. To avoid the expensive pressure solve encountered in a full incompressible Navier-Stokes solve [37], Nicolino et al. [78] modelled the MOSART core using the stream-function/vorticity form of incompressible Navier-Stokes, along with the Boussinesq approximation.

Over the last decade, with increasing availability of computational resources, the use of RANS has gradually become the most common way to conduct these CFD simulations. Zhang et al. [79] used the $k-\epsilon$ model to analyse the steady state operation of an MSR concept with an inlet Reynolds number of 100,000. Cammi et al. [80] employed the $k-\epsilon$ turbulence model within the COMSOL framework for a Reynolds number of 20,000 at the inlet for their 2D model of a single Molten Salt Breeder Reactor core channel, along with a two-group diffusion model for neutronics. They conducted limited verification against similar studies [81] [82] analysing steady-state and transient operation. Fiorina et al. [83] used the $k-\omega$ model to assess the steady-state and transient operation of the Molten Salt Fast Reactor (MSFR) in 2D. Aufiero et al. [84] simulated the MSFR core in 3D to capture the complex flows seen within the core using a coupled neutronics-thermal hydraulics simulation which used $k-\epsilon$ implemented in OpenFOAM. Focusing on neutronics in the proof-of-concept study of their new Multiphysics Object Oriented Simulation Environment (MOOSE) application Moltres, Lindsay et al. [85] performed 2D and 3D coupled neutronics thermal-hydraulics simulations of MSRE-like reactors with a prescribed uniform velocity field that assumes laminar flow due to the MSRE channels having a Reynolds number of 1000 [4]. Podila et al. [33] performed a 3D thermal-hydraulics simulation of a 1/32 radial wedge of the MSRE core, exploiting angular symmetry to reduce computational costs. They used Star-CCM+’s RANS models, namely the Spalart-Allmaras, standard $k-\epsilon$ two-layer, $k-\epsilon$ lag elliptic blending, $k-\omega$ gamma Re-$\theta$, and Reynolds Stress Models (linear pressure-strain two-layer, and elliptic blending models). Podila et al. noticed salt recirculation in the lower plenum and in the upper plenum, above a few graphite stringers. They did not incorporate the pyramid tip at the top of MSRE graphite stringers. While the general trends in fuel salt and graphite temperatures agreed with the MSRE data qualitatively, the absolute values were higher than the MSRE data by about 10 °C.

Depending on the objectives of the study and the verification and validation methodology, these aforementioned
approaches have modelled turbulence in varying levels of detail. However, as Podila et al. [33] have shown, turbulent behaviour can be observed even in laminar regimes due to flow instabilities, as wall-bounded shear flows in reactor channels undergo flow separation in regions such as reactor plena. This can lead to the formation of sustained vortices in the form of individual vortices that trap and recirculate fuel salt or coherent turbulent structures such as quasi-periodic vortex streets (Figure 3) which can create localised hotspots, especially in MSRs which have the fuel dissolved in the carrier salt itself. Vortex streets across channels can interact to form a gap vortex network [35]. Modelling such turbulent flow in reactors requires more sophisticated turbulence models compared to the ones discussed previously. For that reason, we are extending the CFD analysis of the MSRE beyond RANS using Large Eddy Simulation (LES). Such high-fidelity simulations can also contribute to optimising heat transfer and reducing vibrations associated with large scale networks of coherent turbulent structures.

![Vortex street in the wake of a circular cylinder at Re=105 (reproduced from [86]).](image)

Observations made during experiments and high-fidelity simulations aimed at investigating flow instabilities and turbulence in fluids other than molten salts also indicate that turbulent structures can form in compact geometries at relatively low Reynolds numbers. While the experimental data for molten salts are limited, the conclusions from these studies regarding geometry-induced transition to turbulence can be extrapolated to MSRs of similar size operating at comparable Reynolds numbers due to the property of Reynolds number similarity of the Navier-Stokes equations [35]. The high-fidelity simulations discussed below are non-dimensionalised and are focussed entirely on simulating turbulent flow at a certain Reynolds number without incorporating heat transfer. Therefore the results are relevant to any MSR with a similar geometry and comparable Reynolds number. Similarly, for experiments focussed entirely on fluid mechanics without accounting for heat transfer, parallels may be drawn between the experiment and MSRs with similar geometries and Reynolds numbers. According to Bardet and Peterson [87], restrictions on the working fluid in such studies can be relaxed considerably as long as the Reynolds number is matched – even water may be used in the experimental study of the flow of molten salts.
Tatsumi and Yoshimura [88] found that laminar flow in a rectangular duct is unstable above a critical aspect ratio for any fluid, demonstrating the importance of flow geometry in turbulent transitions, in addition to the Reynolds number. The presence of these instabilities contradicts the analytic studies that had previously predicted Poiseuille flow to be linearly stable to small axisymmetric perturbations at all Reynolds numbers [89]. This has led to a search for possible explanations for these transitions and turbulent structures, in order to exercise better control over turbulence in engineering applications.

Gosset and Tavoularis [90] experimentally studied laminar flow in a rectangular channel with a cylindrical rod with water as a working fluid. They found weak pulsations between the rod and the channel wall at a critical Reynolds number. This critical Reynolds number decreased with increasing distance between the rod and the channel wall, exhibiting strong dependence on geometry. The pulsations became more potent with increasing Reynolds number, and developed into hair-pin vortices, then into quasiperiodic laminar vortices on alternating sides of the gap, before finally transitioning into turbulent flow with a quasiperiodical vortical structure. Their work demonstrates the need for studying flow instability at low Reynolds numbers, as the transition to turbulence is determined by instabilities occurring at smaller Reynolds numbers. The instabilities observed at smaller Reynolds numbers often persist at higher Reynolds numbers as well, as seen in the quasi-periodic von Karman vortex streets formed in flows perpendicular to the axis of a cylinder (Figure 3). Gosset and Tavoularis suggest that in narrow gaps, for a given Reynolds number, viscous forces suppress local pulsations, increasing the local critical Reynolds number, while low amplitude pulsations may occur in wider gaps. This narrow region thus creates a low-velocity streak that persists along the entire channel, with a parabolic Poiseuille-like spanwise profile. This resembles the antisymmetric, wake-like profile that is observed in cross flow across cylinders and generates von Karman vortex streets. Gosset and Tavoularis posit that this antisymmetric instability mode is responsible for the quasiperiodicity of the vortices generated.

Within reactor rod bundles, large scale quasiperiodic vortical structures present similar pulsations, increasing momentum and heat transfer between interconnected sub-channels. Rowe et al.[91] found that reducing pitch-to-diameter ratios in light water reactor bundles increases turbulence intensity and the dominant frequency of turbulence. After investigating flow with Reynolds numbers between 50,000 and 200,000, they found the observed turbulence parameters to be largely insensitive to Reynolds number. Möller [92] investigated the aforementioned flow pulsation between light water reactor sub-channels, which drives the mixing process across sub-channels, resulting in a high heat transfer coefficient locally. They suggests it may be a contributing factor in flow-induced vibrations in rod bundles. They also demonstrated that the Strouhal number, which is the nondimensionalised fluctuation frequency associated with oscillating instabilities (such as vortex shedding and periodic von Karman vortex streets), was independent of the Reynolds number above a certain critical Reynolds number but strongly
Ninokata et al. [93] pointed out that while there is an abundance of experimental data for commercial Light Water Reactor (LWR)s with relatively large pitch-to-diameter ratios of 1.3-1.4, newer sodium-cooled fast reactors with pitch-to-diameter ratios 1.08-1.21 and relatively lower Reynolds numbers had not been investigated to the same extent as LWRs. Focusing on assemblies with pitch-to-diameter values representative of such compact reactors, they conducted non-dimensionalised Direct Numerical Simulations (DNS) which produced results indicating the presence of anisotropic turbulent behaviour for relatively low Reynolds number values between 4000-20000. Vortices in turbulence-driven secondary flow can be observed for a Reynolds number of 6000. They found that secondary flow vorticity becomes increasingly concentrated around the pin walls as pitch-to-diameter ratio decreases. With decreasing pitch-to-diameter values, large scale periodic flow oscillations are also expected, and they result in high inter-sub-channel heat and momentum exchanges. They also discovered vortices and oscillations in turbulent flow exchanges between regions of different thickness in highly eccentric annuli, further highlighting the impact of geometry on the formation of turbulent structures across a range of Reynolds numbers. However, they found no stable solutions for low Reynolds number when studying wall shear stress using a $k-\epsilon$ nonlinear model. These results are pertinent to modern nuclear reactor designs that are becoming more and more compact for reasons grounded in neutronics and economics. Channel-type MSRs in which moderating material forming channels or sub-channels for fuel salt could exhibit similar behaviour.

More recently, Proper Orthogonal Decomposition (POD) has been used in order to better understand the mechanisms behind the instabilities observed in compact geometries at low or transitional Reynolds numbers. In POD, the fluctuating velocity field is decomposed in terms of orthonormal eigenfunctions such as Fourier modes [35] [94]. The basis functions are chosen such that the first N modes maximise the energy contained in said modes. Thus, with a few eigenfunctions most of the energy and turbulence characteristics of a flow can be analysed by studying the characteristics of individual modes. Furthermore, reduced order models based on POD eigenmodes instead of a full Navier-Stokes solve may be constructed, reducing computational costs. As an example of the use of POD to analyse turbulence, Merzari et al. [95] observed instabilities in eccentric and U-shaped channels with a narrow gap at Reynolds numbers as low as 3000. They also postulated that the most energetic and unstable POD mode observed in laminar flow, characterised as the propagation of an asymmetric pressure wave in the streamwise direction, is the mode that dominates turbulent structures at high Reynolds numbers, supporting the observations of Gosset and Tavoularis [90].

Von Karman vortex streets [35] were observed by Merzari et al. [71] in an LES of a 37-pin hexagonal lattice rod bundle. Its sub-channels have similarities to channel-type MSR designs. While investigating a lattice typical of advanced reactors at a Reynolds number of 66,000 and a pitch-to-diameter ratio of 1.12, they observed the formation
of vortex streets near the canister wall for sufficiently small ratios of distance between outer pins and canister walls to the channel diameter. The flow in the centre of the domain had characteristics of incoherent turbulence. In the same study, gap vortex streets were observed at the relatively low Reynolds number of 15,000 in an sodium-cooled fast reactor core. They found the flow was edge-channel dominated. In fact, these channels mitigate the vortex street as the peripheral channels have no gap vortex street. These studies clearly demonstrate the effect of geometry and need for simulating flow in large structures such as rod bundles as a whole, instead of individual channels, and for analysing peripheral flow carefully. Their analysis of a 2 × 2 LWR bundle also demonstrated that RANS models underpredict turbulence. However, their study also discusses multiple challenges encountered in such analyses.

In order to identify gap vortex streets through a more quantitative approach, the authors performed POD with regional clipping operators to assess local flow structures. To accomplish this, the authors had to analyse 600 TB of data. Furthermore, as geometries become more and more complex, resolving flow and thermal boundary layers while solving conjugate heat-transfer problems can become prohibitively expensive. For the second challenge, the authors propose a reduced-order model based on POD that exploits the orthonormality of POD basis functions to reduce Navier-Stokes equations to ordinary differential equations. A similar analysis by Merzari and Ninokata found coherent structures in a tight lattice rod bundle for Reynolds numbers of 5500 and 6400.

In a related study, Merzari and Fischer [96] analysed compact rod bundles and found Kelvin-Helmholtz instabilities forming at a relatively low Reynolds number of 3000. Not only did they demonstrate that laminar flow in compact rod bundles is unstable, they also showed that the spacer grids added to rods do not remove this instability and offer limited mitigation of turbulence. They also noted the presence of pulsations in the channel flow.

Hence, there is evidence that indicates that turbulent behaviour may be present in compact light-water and sodium-cooled reactors. These concerns point to the possibility of such turbulent behaviour in small MSRs that have channels or sub-channels for fuel salts. This motivates the investigation the significance of geometry-induced turbulence at low Reynolds numbers in thermal-hydraulics simulations of MSRs using high-fidelity CFD. While RANS models have been applied to MSRs, caution must be exercised when modelling high Reynolds number flows or transition regions, as these models underestimate turbulence and model flows incorrectly, especially in transition regions, near-wall regions, and parts of the reactor where anisotropic turbulence may occur. $k − \epsilon$ models are known to significantly overpredict the rate of spreading for round jets [35], which may be a concern in the upper plena of channel-type MSRs. This motivates investigation of the significance of turbulent phenomena in MSRs with greater accuracy, using LES or DNS. If significant, it is important to analyse the flow parameters, salt properties, and geometries which result in the formation of significant turbulent structures. This will help determine whether RANS is appropriate for the local flow conditions and how different geometry configurations will affect flow velocity and local temperatures.
To that end, we simulated flow around an MSRE stringer using LES. In particular, we studied the effect of the often neglected pyramid top of the graphite stringer on the flow. Our focus was on the investigation of the effects of persistent individual vortices or coherent turbulent structures, also known as quasi-coherent structures [35]. These structures are regions where characteristic coherent patterns like vortices emerge from turbulent flow over time. A more precise, quantitative definition is challenging to formulate, due to the highly random nature of near-wall turbulent phenomena. Historically the study of these structures has been highly dependent on visualisation combined with observing their effects through secondary parameters such as temperature. Our approach is similar, in that we used time averaged data for visualisation and calculation of average velocities and temperatures to detect these vortices and to assess their impact.
Chapter 4

Methodology

This section provides an overview of the simulated reactor, the geometry of interest, and the Computational Fluid Dynamics (CFD) code used for our simulation. The chapter concludes with details of the simulation such as meshing, calculation of source terms, and miscellaneous Nek5000 parameters. All the relevant input data and Nek5000 input files are also available online as a Github repository release [97].

4.1 Molten Salt Reactor Experiment

The Molten Salt Reactor Experiment (MSRE) (Figure 1.2) was an experimental thermal liquid-fuelled molten salt reactor operated from 1965 to 1969 at Oak Ridge National Laboratory (ORNL). The design originated from ORNL’s Aircraft Reactor Experiment designs, as a part of their Aircraft Nuclear Propulsion program [98]. The purpose of the experiment was to demonstrate the viability of molten salt reactors, and to encourage further development of experimental and commercial prototypes. ORNL constructed the reactor in 1964 in the building intended for the Aircraft Reactor Experiment. It was fuelled by 33 % enriched $^{235}\text{U}$ dissolved in the LiF-BeF$_2$-ZrF$_4$ molten carrier salt.

The primary heat exchanger had LiF-BeF$_2$ salt as the secondary coolant salt. Any parts of the reactor in contact with the corrosive molten salts were constructed of Hastelloy-N. The reactor was moderated by graphite (Figs. 1.3-4.3). Compared to the operating pressure of 2175 psig in a Pressurized Water Reactor (PWR) core [18], the MSRE operated at a mere 5 psig due to the high boiling point of the molten salt fuel. This made the design much safer than a PWR. Salt drain tanks provided additional passive safety by reducing the probability of meltdowns (Figure 4.1).

After 9000 equivalent full-power hours of operation with $^{235}\text{U}$, the reactor was operated for over 2500 hours with $^{233}\text{U}$ dissolved in the molten salt, making it the first reactor to be fuelled by $^{233}\text{U}$. The reactor operated safely and without incident. The Hastelloy-N structural components suffered minimal corrosion despite extended contact with corrosive salt and constant irradiation. During operation and decommissioning, the molten salts were handled and reprocessed safely despite their radioactivity and toxicity. Although the reactor was not designed to breed $^{233}\text{U}$ from $^{232}\text{Th}$ (due to economic constraints no blanket salt for breeding purposes was present), the MSRE demonstrated the feasibility of $^{233}\text{U}$-fuelled reactors. For these reasons, the MSRE is an extremely important achievement in nuclear
engineering. It serves as the inspiration for many modern Molten Salt Reactor (MSR) designs. Furthermore, the data from the MSRE is frequently used for validation of neutronics and thermal-hydraulics simulations of MSRs [75, 85, 33]. Currently, an MSRE benchmark is under development for validation of tools for simulating MSRs [99].

Figure 4.1: A diagram of the MSRE primary loop [3]).
The salient features of the primary loop pertaining to this thesis are briefly discussed here. The reactor vessel was connected to a primary heat-exchanger cooled by the coolant salt. A secondary air-cooled heat exchanger removed heat from the primary heat-exchanger (Figure 4.1). The reactor vessel was connected to drainage tanks underneath it that were blocked by a freeze valve or a freeze plug. This valve prevented drainage of fuel salt from the reactor under normal operation using frozen salt (created by air-cooling a section of the freeze plug externally) that blocked the drainage valve. However, in case of overheating or loss of power, the salt within the freeze plug would melt, allowing drainage of the fuel salt into air-cooled, subcritical tanks. The reactor also had a helium sparging system to remove $^{135}$Xe, which is a potent neutron poison that must be removed to maintain neutron economy. A fuel storage and reprocessing system was also available to manage the fuel composition, removal of fission products, and to study the properties of the fuel salt. All pipes and reactor components with circulating molten salts were heated electrically to ensure the molten salt did not freeze and create blockages [3].

The fuel salt entered the space between the inner "core can" and the outer core vessel through a flow distributor near the top of the reactor vessel, after which it flowed turbulently down the circumference of the can in a downward
spiral (Figures 1.3 and 4.2). The fuel salt then entered the core can at the bottom where it encountered 48 anti-swirl vanes, each 11 in. long, positioned at the bottom of the vessel, extending from the periphery of the can towards its centre. These vanes were designed to remove the rotational flow of the salt and to mitigate salt entrainment and recirculation zones. The salt continued upwards through a graphite matrix composed of long, cuboidal 67 in. × 2 in. × 2 in. graphite bars or stringers with pyramidal tips. Note that the distance from the beginning of the channel to the stringer-tip was 63 in., and the remaining 4 in. were embedded in mounts. This section of the stringer is also the focus of our simulations. The tips were designed to prevent stagnation of fuel salt on top of the stringers when the reactor was drained [3]. A total of 1140 salt channels were present in this graphite core. Salt from these channels emerged into an upper plenum from where it exited the reactor vessel.

Due to computational limitations, we simulated the salt flow in channels around one graphite stringer, and a small section of the plenum above it. We did not model anisotropic heat conduction and neglected axial conduction along the channel as most of the heat transfer between the stringer and the salt is radial, in the channel. Important reactor parameters used in the simulation are described in Table 4.1.
Table 4.1: MSRE Data used for simulation.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fuel Salt</td>
<td>LiF(65)-BeF₂(29.1)-ZrF₄(5)-UF₄(0.9)</td>
<td></td>
<td>TM-728 [3]</td>
</tr>
<tr>
<td>Flow rate</td>
<td>1200</td>
<td>gpm</td>
<td>TM-728 [3]</td>
</tr>
<tr>
<td>Channel flow rate</td>
<td>1</td>
<td>gpm</td>
<td>TM-728 [3]</td>
</tr>
<tr>
<td>Inlet Pressure</td>
<td>20</td>
<td>psig</td>
<td>TM-728 [3]</td>
</tr>
<tr>
<td>Outlet Pressure</td>
<td>35</td>
<td>psig</td>
<td>TM-728 [3]</td>
</tr>
<tr>
<td>Salt Density</td>
<td>141</td>
<td>lb/ft³</td>
<td>TM-3229 [4]</td>
</tr>
<tr>
<td>Inlet Temperature</td>
<td>1175</td>
<td>°F</td>
<td>TM-728 [3]</td>
</tr>
<tr>
<td>Outlet Temperature</td>
<td>1200</td>
<td>°F</td>
<td>TM-728 [3]</td>
</tr>
<tr>
<td>Max. Outlet Temperature</td>
<td>1260</td>
<td>°F</td>
<td>TM-728 [3]</td>
</tr>
<tr>
<td>Specific Heat Cₚ</td>
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<td>Btu/lb °F</td>
<td>TM-3229 [4]</td>
</tr>
<tr>
<td>Salt thermal conductivity</td>
<td>0.83</td>
<td>Btu/ft °F</td>
<td>TM-3229 [4]</td>
</tr>
<tr>
<td>Graphite thermal conductivity</td>
<td>13</td>
<td>Btu/ft °F</td>
<td>TM-3229 [4]</td>
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<td>Viscosity</td>
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<td>lbs/ft h</td>
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<tr>
<td>Prandtl Number</td>
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<td></td>
<td>TM-3229 [4]</td>
</tr>
<tr>
<td>Channel Reynolds Number</td>
<td>1000</td>
<td></td>
<td>TM-3229 [4]</td>
</tr>
<tr>
<td>Peak fuel power density</td>
<td>31</td>
<td>W/cm³</td>
<td>TM-728 [3]</td>
</tr>
<tr>
<td>Peak fuel power density</td>
<td>14</td>
<td>W/cm³</td>
<td>TM-728 [3]</td>
</tr>
<tr>
<td>Graphite Mean Temperature</td>
<td>1229</td>
<td>°F</td>
<td>TM-728 [3]</td>
</tr>
</tbody>
</table>

4.2 Nek5000

Nek5000 is an open source, highly-scalable spectral elements solver developed for Computational Fluid Dynamics (CFD) applications at Argonne National Laboratory [34]. It is capable of Direct Numerical Simulations (DNS) and Large Eddy Simulation (LES), and has more recently incorporated Reynolds-Averaged Navier Stokes (RANS) models within its framework[100]. The code has been verified and validated [101, 102]. It has also been incorporated into the US Department of Energy’s Nuclear Energy Advanced Modeling and Simulation Workbench [103]. It is often used as a source of high-fidelity CFD data for verifying other CFD codes.

Nek5000’s incompressible Navier-Stokes solver is based on the pressure correction formulation derived from the Uzawa algorithm(Section 2.3). The equations are solved through a hybrid multigrid Schwarz method [104]. High order time steppers such as BDFk/EXTk [37] are used. Nek5000 also offers variable time-stepping to automatically adjust time step size Δt for stability. Nek5000 offers the explicit modal filter [105] and the high pass filter with relaxation term (HPFRT) [106]. Both are comparable in their efficacy. We use the former in our simulations. The explicit modal filter improves upon the performance of a sharp cut-off spectral filter, which can pollute low wavenumber modes over a domain [46]. The modal basis filter is based on the modal basis of Boyd [107], which improves the alignment of filtered functions with boundary conditions. This modal basis comprised of N Legendre polynomials, \( L_k(\xi) \), is given by

\[
\phi_0 = \frac{1 - \xi}{2} \tag{4.1}
\]
\[ \phi_1 = \frac{1 + \xi}{2} \]  
(4.2)

\[ \phi_k = L_k(\xi) - L_{k-2}(\xi), \; k \in [2, N]. \]  
(4.3)

where

\[ k \in [1, N] \]  
(4.4)

\[ \xi = \text{arbitrary independent variable.} \]  
(4.5)

The key idea of the modal filter is to interpolate the velocity function to this new basis, use a spectral filter over this new expansion, and to transform the interpolated and filtered velocity back to the original basis. The mapping to the new modal basis is given by

\[ v(\xi_i) = \sum_{k=0}^{N} \hat{v}_k \phi_k(\xi_i) \]  
(4.6)

\[ v = \Phi \hat{v} \]  
(4.7)

\[ \Rightarrow \hat{v} = \Phi^{-1} v. \]  
(4.8)

The diagonal matrix \( T \) is then applied to \( \hat{v} \) as a filter. Its elements are given by

\[ T_{kk} = \frac{1}{1 + \left( \frac{k}{k_c} \right)^2} \]  
(4.9)

where

\[ k_c = \text{cutoff wavenumber corresponding to } T_k = 1/2. \]  
(4.10)

Therefore, the filtered velocity is

\[ \tilde{v} = \Phi T \Phi^{-1} v. \]  
(4.11)

Nek5000 uses its own mesh formats (.rea and .re2) and has its own mesh generating tools. It also includes tools to convert Exodus or Gmsh’s .msh [108] files to a supported format. Like most spectral codes, Nek5000 uses quadrilateral or hexahedral meshes because directional matrix operators can be cleanly separated along each axis of each element and then used in matrix-free tensor contractions which offer substantial computational advantages over triangular or tetrahedral mesh-based low order finite element solvers(Section 2.2.2).
4.3 Simulation Setup

The following section discusses the geometry meshed, and the parameters used in our Nek5000 simulations.

4.3.1 Meshing and boundary conditions

As discussed previously, our focus is on simulating the flow around and above a graphite stringer of the MSRE (Figure 4.3). The geometry of interest is shown below (Figure 4.4 and 4.5).

Figure 4.4: Top view of an MSRE graphite stringer (shaded) with four salt channels around it. The meshed geometry is highlighted by the red box. The dimensions of the highlighted region are 2 in. × 2 in., as shown in Figure 4.7 (reproduced from [3]).

The meshes for the graphite stringer and the fluid domain around and above it were prepared in Gmsh [108] (Figures 4.8 - 4.7), converted from the original tetrahedral to a Nek5000-supported hexahedral format, and subsequently merged into one mesh file using Nek5000’s post-processing capabilities. During meshing, we paid special attention to element sizes and aspect ratios, as the Spectral Element Method (SEM), like other p-type finite elements, requires fewer elements and relies more on increasing the polynomial order (Section 2.2.2). Compared to h-type Finite Element Method (FEM) solvers, coarser elements are necessary to avoid over-refinement in SEM. However, the downside of larger elements is that poor quality anisotropic elements can cause convergence issues more easily [104]. In general, we maintained an average aspect ratio of around 8-12 across both the graphite (solid domain) and the molten salt (fluid domain) meshes.
Figure 4.5: Top view of an MSRE fuel channel. The shaded portion is graphite. Dimensions are in inches (reproduced from [3]).

Figure 4.6: Top view of the graphite stringer mesh without any deformation. The cross section is 2 in. × 2 in. The original geometry is shown in Figure 4.4.

The inlet was defined at the bottom of the 63 in. long channel. The lower plenum was neglected because of the flow-stabilisation offered by the anti-swirl vanes in the lower plenum [3] and the graphite matrix itself. To
Figure 4.7: Perspective view of the 63 in.-long graphite stringer mesh without any deformation. The original geometry is in Figure 4.3.

Figure 4.8: Top view of the fluid domain mesh without any deformation. The plenum's mesh is conformal to the stringer's mesh in the X-Y plane to allow for merging through PreNek [34]. The cross section is 2 in. × 2 in. The original geometry is shown in Figure 4.4.

study the effect of different stringer tip shapes, we made a base mesh that neglects the pyramidal tip and has a flat surface at the top of a full-length stringer. The mesh was then deformed using Nek5000’s pre-processing capabilities (Appendix C) to three different apex half-angles (Figure 4.10) for the tip. We chose 30°, 45°, and 60°, based on likely machining limitations of the era. This resulted in four meshes - one with the flat top, and three with the aforementioned apex half-angles. The plenum height near the outlet was estimated from a to-scale figure from
Figure 4.9: Perspective view of the 70 in.-long fluid domain mesh without any deformation. The original geometry is shown in Figures 4.2 and 4.3.

Based on this estimate, the outlet was assumed to be 7in. above the stringer’s top, corresponding to a stringer near the centre of the core.

The mesh was non-dimensionalised by scaling it with the reciprocal of the hydraulic diameter, in inches. At the inlet, we used recycle boundary conditions [109] for the velocity and temperature, in which the flow near the inlet was rescaled and recycled to the inlet over successive time steps to rapidly improve the accuracy of the inlet velocity and temperature profiles. The turbulent outflow boundary condition [110] was used to remove recirculation-related instabilities near the outlet. This boundary condition adds divergence in the last layer of the mesh near the outlet to artificially create the effect of a nozzle without actually deforming the mesh, preventing catastrophic backflow near the outlet. We set periodic boundary conditions for both the velocity and temperature field around the stringer and the plenum, to create a unit-cell type model that approximates the aggregate flow in the plenum in the MSRE core as the flow above a stringer interacts with the radially inward flow towards the outlet in the domed plenum. This was done chiefly due to computational limitations that forced us to simulate the flow around just one stringer. One drawback of this approach is that we cannot simulate the effect of the domed plenum on the flow. Meshing data and boundary conditions are summarised in Table 4.2.
Figure 4.10: Exploded view of the MSRE stringer tip, showing the apex half-angle $\theta$ that we varied.

Table 4.2: Mesh dimensions and boundary conditions used in our simulations.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Channel length</td>
<td>1.2 in.</td>
</tr>
<tr>
<td>Channel breadth</td>
<td>0.4 in.</td>
</tr>
<tr>
<td>Stringer length</td>
<td>2 in.</td>
</tr>
<tr>
<td>Stringer breadth</td>
<td>2 in.</td>
</tr>
<tr>
<td>Stringer height</td>
<td>63 in.</td>
</tr>
<tr>
<td>Plenum height</td>
<td>7 in.</td>
</tr>
<tr>
<td>Channel hydraulic diameter</td>
<td>0.624 in.</td>
</tr>
<tr>
<td>Non-dimensional mesh length</td>
<td>112.18 [-]</td>
</tr>
<tr>
<td>Stringer top shape</td>
<td>Flat</td>
</tr>
<tr>
<td></td>
<td>Pyramid (30°)</td>
</tr>
<tr>
<td></td>
<td>Pyramid (45°)</td>
</tr>
<tr>
<td></td>
<td>Pyramid (60°)</td>
</tr>
<tr>
<td>Inlet boundary condition</td>
<td>Recycle condition</td>
</tr>
<tr>
<td>Outlet boundary condition</td>
<td>Turbulent outflow condition</td>
</tr>
<tr>
<td>Mesh walls' boundary condition</td>
<td>Periodic condition</td>
</tr>
<tr>
<td>Velocity initial condition</td>
<td>$v_z = 1$ (non-dimensionalised velocity)</td>
</tr>
<tr>
<td>Temperature initial condition</td>
<td>$T = 0$ in salt</td>
</tr>
<tr>
<td></td>
<td>$T = \frac{1}{2}[1 - \cos(\pi \frac{z - z_1}{z_2 - z_1})]$ in graphite</td>
</tr>
<tr>
<td></td>
<td>($z_1$ &amp; $z_2$ are the $z$ coordinates of the inlet and the outlet respectively)</td>
</tr>
</tbody>
</table>

4.3.2 Simulation Parameters

This discussion focusses on the Boussinesq approximation used in the momentum equation, the volumetric heat source term used in the temperature equation, and other simulation parameters used in our analysis.
**Boussinesq approximation term**

For the momentum equation (Equation 2.21), the non-dimensionalised body-force term is calculated by Nek5000 as

\[
f = \frac{\bar{f} L_c}{U^2}
\]

\[
= \frac{\rho}{\rho(T)} \frac{g L_c}{U^2}
\]

where

\[
g = \text{acceleration due to gravity \([m s^{-2}]\).}
\]

(4.15)

The density in the numerator, \(\rho\), is supplied by Nek5000 when it automatically multiplies the body force term with \(\rho\). We introduce the Boussinesq approximation along the length of the channel by writing \(\rho(T)\) in the denominator as a function of temperature

\[
\rho(T) = \rho_{in}[1 - \alpha(T - T_{in})]
\]

(4.16)

(4.17)

where

\[
\rho_{in} = \text{salt’s density at the inlet \([kg m^{-3}]\)}
\]

(4.18)

\[
\alpha = \text{salt’s isobaric thermal expansivity \([kg m^{-3} K^{-1}]\)}
\]

(4.19)

\[
T_{in} = \text{inlet temperature\([K]\).}
\]

(4.20)

(4.21)

An empirical relationship also exists for molten salts [111], given by

\[
\rho = \bar{\rho} - aT
\]

(4.22)

where

\[
\bar{\rho} = \text{user-defined reference value for density \([kg m^{-3}]\)}
\]

(4.23)
\[ a = \text{empirical constant} \ [kg \ m^{-3} \ K^{-1}] . \] (4.24)

We can deduce \( \tilde{\rho} \) and \( a \) using the empirical model (Equation 4.22) and appropriate salt density data [112] using the salt that resembles the MSRE fuel’s properties most closely. The thermal expansivity can thus be expressed as

\[
\alpha = \frac{1}{V} \left( \frac{dV}{dT} \right)_p = -\frac{1}{\rho} \frac{d\rho}{dT} \tag{4.25}
\]

\[
= \frac{a}{\tilde{\rho} - aT} \tag{4.26}
\]

\[
= \frac{a}{\tilde{\rho} - a(T_{in} + \theta \Delta T)} \tag{4.27}
\]

where

\[
\theta = \text{non-dimensionalised temperature from Equation 2.21}[-]. \tag{4.28}
\]

Using Equations 4.17 and 4.27 in Equation 4.14, we can write

\[
f = \rho g \frac{L_c}{U^2 \rho_{in}[1 - \alpha(T - T_{in})]} \tag{4.29}
\]

Therefore, the Boussinesq term is calculated dynamically using the latest local temperature \( \theta \) at each time step.

**Volumetric heat source term**

For the temperature equations, we approximated the volumetric source term \( \tilde{q}''''_s(z) \) in the molten salt as a sinusoid within the channel, and as a linearly decreasing function within the plenum.

\[
\tilde{q}''''_s(z) = \begin{cases} 
q_{s0}(\epsilon \sin \pi \hat{z}), & \forall z \in (z_1, z_2) \\
q_{s0}(mz + c), & \forall z \in (z_2, z_3) 
\end{cases} \tag{4.30}
\]

where

\[
q_{s0} = \text{peak value of the volumetric heat source in the salt} \ [W \ m^{-3}] \tag{4.31}
\]

\[
\epsilon = \text{arbitrary non-zero constant}[-] \tag{4.32}
\]

\[
\hat{z} = \frac{z - z_1}{z_2 - z_1} [-] \tag{4.33}
\]
\[ m = \frac{\epsilon}{z_2 - z_3} \quad [\text{-}] \quad (4.34) \]
\[ c = \frac{\epsilon z_3}{z_3 - z_2} \quad [\text{-}] \quad (4.35) \]
\[ z_1 = \text{non-dimensionalised inlet z-coordinate} [-] \quad (4.36) \]
\[ z_2 = \text{non-dimensionalised top-of-the-channel z-coordinate} [-] \quad (4.37) \]
\[ z_3 = \text{non-dimensionalised outlet’s z-coordinate} [-]. \quad (4.38) \]

Setting the average over \( z \) of the source term to one, we obtain the amplitude \( q_0 \):

\[ \int_{z_1}^{z_3} \tilde{q}''' \, dz = 1 \quad (4.39) \]

\[ \Rightarrow q_{s0} = \frac{1}{\frac{2\pi}{\epsilon} + \frac{m}{2} (z_3 + z_2) + c}. \quad (4.40) \]

Since the average is one, we can scale the amplitude \( q_{s0} \) by a constant \( q_s^{av} \) to adjust the average of the source term to match the MSRE data. In doing this, we obtain:

\[ \tilde{q}_{s0} = q_{s0} q_s^{av} \quad (4.41) \]

\[ \Rightarrow \tilde{q}_s'''(z) = \begin{cases} \tilde{q}_{s0}(\epsilon + \sin(\pi \hat{z})), & \forall z \in (z_1, z_2) \\ \tilde{q}_{s0}(mz + c), & \forall z \in (z_2, z_3) \end{cases} \quad (4.42) \]

where

\[ q_s^{av} = \text{scaling constant for the salt’s source term} \quad [-]. \quad (4.43) \]

In Equation 2.3, the non-dimensionalised source is

\[ q_s''' = \frac{L_c}{\rho c_p U \Delta T} \tilde{q}_s''' \quad (4.44) \]

The source term in the graphite \( \tilde{q}_g'''(z) \) can be represented by a simple sinusoid

\[ \tilde{q}_g''' = q_{g0} \sin(\pi \hat{z}) \quad (4.45) \]

Similar to the procedure employed for the salt’s source term, we can set the average of the graphite source term to one to obtain \( q_{g0} = \pi / 2 \). We can then scale the overall average of the source term using the scaling factor \( q_g^{av} \).
yielding the expressions

\[
\tilde{q}_g = q_{g0} q_{g}^{av} \quad (4.46)
\]

\[
\Rightarrow \tilde{q}_g'' = \tilde{q}_{g0} \sin \pi \hat{z} \quad (4.47)
\]

where

\[
q_{g0} = \text{peak value of the volumetric heat source in the graphite [W m}^{-3}] \quad (4.48)
\]

\[
q_{g}^{av} = \text{scaling constant for the salt's source term [-].} \quad (4.49)
\]

The non-dimensionalised source term for graphite is

\[
q_g'' = \frac{L_c}{\rho C_p U \Delta T} \tilde{q}_g''. \quad (4.50)
\]

The data used for the source and the Boussinesq terms are summarised in Table 4.3. As we are simulating a channel close to the core’s centre, we are matching the peak values of the heat source terms to the MSRE data. For a channel near the core’s centre, the average scaling factor for the heat source term will be higher than the overall core’s average source term value, as expected.

Table 4.3: Parameters used to calculate the Boussinesq and heat source terms.

<table>
<thead>
<tr>
<th>Term</th>
<th>Definition</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>U</td>
<td>Average velocity in channel [4]</td>
<td>0.22 ms(^{-1})</td>
</tr>
<tr>
<td>(\rho_{in})</td>
<td>Density at inlet [3, 111]</td>
<td>2266.9 kg m(^{-3})</td>
</tr>
<tr>
<td>(\bar{\rho})</td>
<td>Density from Equation 4.22 [111]</td>
<td>2811.82 kg m(^{-3}) [112]</td>
</tr>
<tr>
<td>a</td>
<td>Empirical constant from Equation 4.22[111]</td>
<td>0.6 kg m(^{-3}) K(^{-1}) [112]</td>
</tr>
<tr>
<td>(\Delta T)</td>
<td>For non-dimensionalisation (Equation 2.21)</td>
<td>1 K</td>
</tr>
<tr>
<td>(\epsilon)</td>
<td>Constant from Equation 4.30</td>
<td>0.01</td>
</tr>
<tr>
<td>(z_1)</td>
<td>Inlet z-coordinate</td>
<td>-62 in</td>
</tr>
<tr>
<td>(z_2)</td>
<td>Top-of-stringer z-coordinate</td>
<td>1 in</td>
</tr>
<tr>
<td>(z_3)</td>
<td>Outlet z-coordinate</td>
<td>8 in</td>
</tr>
<tr>
<td>(\tilde{q}_{s0})</td>
<td>Salt heat source peak value</td>
<td>31 W cm(^{-3})</td>
</tr>
<tr>
<td>(q_{s}^{av})</td>
<td>Salt heat source average value</td>
<td>20 W cm(^{-3})</td>
</tr>
<tr>
<td>(\tilde{q}_{g0})</td>
<td>Graphite heat source peak value</td>
<td>0.979 W cm(^{-3})</td>
</tr>
<tr>
<td>(q_{g}^{av})</td>
<td>Graphite heat source average value</td>
<td>0.623 W cm(^{-3})</td>
</tr>
<tr>
<td>N.A.</td>
<td>MSRE Salt heat source peak value [3]</td>
<td>31 W cm(^{-3})</td>
</tr>
<tr>
<td>N.A.</td>
<td>MSRE Salt heat source average value [3]</td>
<td>14 W cm(^{-3})</td>
</tr>
<tr>
<td>N.A.</td>
<td>MSRE Graphite heat source peak value [3]</td>
<td>0.98 W cm(^{-3})</td>
</tr>
<tr>
<td>N.A.</td>
<td>MSRE Graphite heat source average value [3]</td>
<td>0.34 W cm(^{-3})</td>
</tr>
</tbody>
</table>
Nek5000 parameters

Nek5000 parameters essential for performing the simulation are listed in Table 4.4. The theoretical background for these parameters has been presented in Chapter 2. Note that the average velocity in the channel was computed from data presented in Tables 4.1 and 4.2 and the formula

\[ Re = \frac{\rho U D_h}{\mu} \]  \hspace{1cm} (4.51)

where

\( Re = \) Reynolds number in channel [-] \hspace{1cm} (4.52)
\( \rho = \) molten salt density [kg m\(^{-3}\)] \hspace{1cm} (4.53)
\( U = \) average velocity [m s\(^{-1}\)] \hspace{1cm} (4.54)
\( D_h = \) hydraulic diameter of channel [m] \hspace{1cm} (4.55)
\( \mu = \) molten salt viscosity [Pa·s]. \hspace{1cm} (4.56)

The convective time unit is given by

\[ t = \frac{D_h}{U} \]  \hspace{1cm} (4.57)

where

\( D_h = \) hydraulic diameter [m] \hspace{1cm} (4.58)
\( U = \) average velocity [m s\(^{-1}\)]. \hspace{1cm} (4.59)
Table 4.4: Simulation parameters used across all MSRE simulations.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Domain dimension</td>
<td>3D</td>
</tr>
<tr>
<td>Gauss-Lobatto Legendre points per element per direction</td>
<td>8</td>
</tr>
<tr>
<td>Gauss-Lobatto points for dealiasing</td>
<td>12 (Section 2.3)</td>
</tr>
<tr>
<td>Gauss-Lobatto Legendre points for pressure</td>
<td>8 (Section 2.3)</td>
</tr>
<tr>
<td>Average velocity in channel</td>
<td>0.2194 m s$^{-1}$</td>
</tr>
<tr>
<td>Convective time unit</td>
<td>0.0722 [-]</td>
</tr>
<tr>
<td>End time</td>
<td>180 s (physical time)</td>
</tr>
<tr>
<td>Flow-through time</td>
<td>112 s (physical time)</td>
</tr>
<tr>
<td>Start of time-averaging</td>
<td>112 s (physical time)</td>
</tr>
<tr>
<td>Time-averaging duration</td>
<td>68 s (physical time) or 941.3 (convective time units)</td>
</tr>
<tr>
<td>Time stepper</td>
<td>BDF2 [37]</td>
</tr>
<tr>
<td>Variable timestepping</td>
<td>Enabled</td>
</tr>
<tr>
<td>Target CFL</td>
<td>0.5</td>
</tr>
<tr>
<td>Filter</td>
<td>Explicit modal filter [105]</td>
</tr>
<tr>
<td>Filter Weight</td>
<td>0.05</td>
</tr>
<tr>
<td>Filtered Modes</td>
<td>2.0</td>
</tr>
<tr>
<td>Pressure residual tolerance</td>
<td>$10^{-5}$</td>
</tr>
<tr>
<td>Residual projection</td>
<td>Enabled</td>
</tr>
<tr>
<td>Velocity residual tolerance</td>
<td>$10^{-6}$</td>
</tr>
<tr>
<td>Temperature residual tolerance</td>
<td>$10^{-6}$</td>
</tr>
</tbody>
</table>
Chapter 5

Results and Discussion

In this chapter, we present the Large Eddy Simulation (LES) results of our Molten Salt Reactor Experiment (MSRE) simulations. We explain the qualitative properties of the flow and the quantitative differences in the flow and temperatures across the four geometries. We investigate where these differences stem from and assess the impact of the geometry on these differences. The discussion explores the significance of these results in relation to typical Computational Fluid Dynamics (CFD) analyses of the MSRE and other channel-type Molten Salt Reactors (MSRs).

5.1 Results

We analysed the output data from Nek5000 using a combination of visualisation and averaging. Visualisation provides a qualitative understanding of the flow and its effects on the temperature, whereas the averaged metrics provide quantitative insights into the mechanisms affecting the flow. Key features common to all plots are that all units are SI units and any vector arrows are not to scale – they are indicative of the direction of the flow alone. For quantitative metrics, note that the negative velocity values in the velocity plots indicate backward flow or recirculation. The maximum temperature values were obtained at the last time step from our simulations. The simulations converged in velocity up to \(10^{-6}\). The temperature also converged; the mean temperature changed by less than 1% at the final time-step, and the maximum temperature by less than 0.1%.

The first set of plots examines the z-velocity and temperature using a pseudocolour plot to verify that the model is working as intended. Figures 5.1 and 5.2 show the flow inside the channels around an MSRE graphite stringer. As expected, the flow is laminar in the channel, with the highest velocity in the middle of the four half-channels, and the lowest velocity is near the channel wall due to shear. The latter is where the maximum temperature in the channel is also observed (Figure 5.3) – the salt with the fuel dissolved in it is moving extremely slowly in the boundary layer, and due to poor heat transfer observed in laminar flow the salt in the boundary layer heats up more than the salt in the middle of the channel.

The next set of pseudocolour plots (collectively Figure 5.4) focus on the flow in the plenum, showing a 2D slice through the Y axis (i.e. viewed in the XZ plane) at the last time-step. These plots demonstrate the presence of
Figure 5.1: The z-velocity [m s$^{-1}$] in the XY plane (top view) inside the MSRE channel. The 2D slice was obtained near the top of the channel. The four salt channels end near the green and light blue regions, whereas the graphite is in deep blue. The original geometry is shown in Figure 4.4.
Figure 5.2: The z-velocity \([\text{m s}^{-1}]\) in the XZ plane (side view) inside the MSRE channel. The section shown is four inches long, near the top of the channel. The salt channel is in the middle, ending in the green and light blue regions. The graphite is shown in deep blue. The original geometry is shown in Figures 4.2 and 4.3.
Figure 5.3: The temperature [K] in the XY plane (top view) inside the MSRE channel. The 2D slice was obtained near the top of the channel. The four salt channels end near the red and green regions. The graphite is in deep blue and light blue – the former mostly near the colder centre and the latter near the warmer edges close to the hot salt channels. The original geometry is shown in Figure 4.4.
turbulent vortices due to flow separation near the top of the stringer, in the salt’s transition from the channel to plenum. The plots also qualitatively confirm that the turbulent flow in the upper plenum is affecting both velocity and temperature, and to different degrees for different tip shapes. The edges of the plots show the jets from the four half channels reaching the outlet after going through some mixing, but on average, preserving much of their profile upon exiting the channel. This mixing can also be seen in Figure 5.5. The inward boundary layers from these four jets also separate near the outlet and form large recirculation zones where the salt is trapped in four large vortices. The shape of the tip also impacts the way in which flow separation occurs immediately near the tip, creating smaller vortices around the tip as the salt jet emerges from the straight channel. Much of the following discussion focusses on the interplay between the larger recirculation vortices that are set up in the plenum, the smaller eddies formed near the tip due to flow separation, and how that affects the average temperatures of the graphite’s top surface and the salt in the plenum.

We visualised the data at each time step and observed the salt trapped in these recirculation zones. The vortices in these regions persist for the entire duration of the time-averaging period from \( t = 112 \) s to 180 s. Every 10 s or so minor disruptions of these vortices or formation of secondary vortices also occur. These vortices last long enough that they are clearly visible in our time-averaged data (Figures 5.6 and 5.7). After observing these vortices, our first concern was whether the salt trapped in the vortices ever gets to dangerous temperatures where it could boil the salt (\( \approx 1673 \text{ K} \) [113]). As discussed previously, the simulations are nearly steady-state in temperature, therefore the maximum temperature observed is at the final-time step. The values and locations of the temperature maxima are recorded in Table 5.1. For reference, the stringer extends from \( z \in [-62, 1] \) inches and the plenum from \( z \in (1, 8] \) inches. The maximum temperature is similar across the four cases, well within the standard operating conditions recorded for the MSRE [3], and nowhere close to dangerous levels. The locations of the temperature maxima are also similar, existing within the channel’s boundary layer where the salt is moving the slowest. The \( z \)-coordinates of the maxima are about 24 in. above the centre-line of the stringer because although the source term peaks in the middle of the graphite channel, upward advection coupled with buoyancy from shifts the location of the actual maximum significantly above the centre of the graphite. This is also in qualitative agreement with the findings of Podila et al. [33]. The results demonstrate that changes in tip shape do not create recirculation vortices in the plenum that get hotter than the salt in the channel. This is to be expected, since the MSRE was a small, stable test-reactor that operated without incident, and small perturbations to its geometry should not destabilise the reactor to the extent of making the plenum hotter than the interior of the channel, where most of the fission is occurring (see the source term in Equation 4.30).

However, Figure 5.4 qualitatively demonstrates that the tip-shape has a non-trivial impact on the flow in the plenum. We conducted a comparative analysis to investigate the effects of different stringer geometries on the salt
Figure 5.4: Side-view (XZ plane) of the $z$-velocity [m s$^{-1}$] in the plenum at the last time step. The Reynolds number is 1000 for the flow within the channel. The region without vector arrows is the graphite, the rest is the molten salt. Vector arrows not scaled to magnitude. Turbulent behaviour due to flow separation is visible. See Figure 4.3 for original geometry.
Figure 5.5: Top view (XY plane) of the time-averaged $z$-velocity [m s$^{-1}$] in the plenum near the outlet (i.e. the entire plot shows molten salt and no graphite). Partially-mixed jets from the MSRE half-channels are visible.
Table 5.1: Maximum temperature in the entire domain.

<table>
<thead>
<tr>
<th>Case</th>
<th>Value(K)</th>
<th>Location (in.)</th>
</tr>
</thead>
<tbody>
<tr>
<td>30°</td>
<td>943.0254</td>
<td>(-0.999, 0.505, -6.645)</td>
</tr>
<tr>
<td>45°</td>
<td>943.0256</td>
<td>(-0.999, -0.505, -6.644)</td>
</tr>
<tr>
<td>60°</td>
<td>943.0247</td>
<td>(-0.999, -0.505, -6.639)</td>
</tr>
<tr>
<td>90° (flat)</td>
<td>943.0245</td>
<td>(0.505, -0.999, -6.621)</td>
</tr>
</tbody>
</table>

To separate random fluctuations with trivial effects from the impact of more sustained vortices, we time-averaged the velocity and temperature output from Nek5000 for every node on the mesh. We performed time-averaging after one flow-through time, i.e. after the salt had travelled the length of the domain once. For our simulations, this time was $t=112$ s. Time-averaging was then performed from $t=112$ s until the end of the simulation at $t=180$ s, for a duration of 68 s or 941.3 convective time units (Table 4.4). Using these time-averaged data, we used a combination of visual inspection and spatial averaging to assess the impact of the tip-shape and the relative significance of the effects. The data are plotted in Figures 5.5, 5.6 - 5.8. These plots help visualise the nature of the vortices formed, their direction, and the extent of mixing of the hot channel jets with the colder salt in the plenum.

The quantitative analysis of these averaged data is summarised in Tables 5.3, 5.2, and 5.4. These tables include the maximum and minimum values of $z$-velocity in the plenum, and volumetric averages of $z$-velocity in the plenum and around the tip. The average velocity and temperature for plenum are calculated from the salt volume extending from the end of the straight channel to the height of five hydraulic diameters below the outlet. The average temperature and velocity for the salt near the tip are from the volume of salt between the end of the straight channel to the top of the pyramid in case of the pyramid-tipped stringers, and from the top of the stringer to one hydraulic diameter above the stringer in the flat-top case. The trends that emerge from these data are plotted in Figures 5.9, 5.10, and 5.11. Note that the ranges of variation in the average temperatures of the plenum salt, the salt around the tip, and the graphite top are 2.54 K, 1.82 K, and 1.76 K respectively (Table 5.2).

Table 5.2: Time and spatial averages of temperatures around graphite tip. The data were averaged for 68s or 941.3 convective time units.

<table>
<thead>
<tr>
<th>Case</th>
<th>Salt temperature in plenum Volumetric average (K)</th>
<th>Salt temperature around tip Volumetric average (K)</th>
<th>Graphite top temperature Surface average (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>30°</td>
<td>919.03834</td>
<td>917.81988</td>
<td>913.31320</td>
</tr>
<tr>
<td>45°</td>
<td>918.61431</td>
<td>916.71073</td>
<td>911.55268</td>
</tr>
<tr>
<td>60°</td>
<td>921.15900</td>
<td>918.5263</td>
<td>912.20180</td>
</tr>
<tr>
<td>90° (flat)</td>
<td>919.36498</td>
<td>917.1199</td>
<td>912.61204</td>
</tr>
</tbody>
</table>
Figure 5.6: Velocity streamlines along with a transparent 3D pseudocolour plot of the time-averaged z-velocity [m s$^{-1}$] in the plenum. The streamlines start right above the top of the graphite and extend to the outlet (see Figure 4.3 for original geometry).

The relative magnitudes of the volumetric averages of velocity are not only a measure of the speed of the flow but also the turbulence in a particular region. This is because of negative z-velocity values present in vortices where recirculation is occurring and the direction of the velocity is changing. In regions where these vortices are strong, the velocity is often negative, reducing the volumetric average velocity. Therefore, a reduction in volumetric average
Figure 5.7: Side view (XZ plane) of the time-averaged z-velocity [m s$^{-1}$] in the plenum. The region without vector arrows is the graphite, the rest is the molten salt. See Figure 4.3 for original geometry.

velocity represents *either* more turbulent flow or the flow slowing down without turbulence. The maximum and minimum velocities are less important than the average velocity as they are local metrics. However, in conjunction with the trends seen in the average velocity and temperature values, the velocity extrema provide some insights into the nature of the flow and the magnitude of turbulence.
Figure 5.8: Side view (XZ plane) of the time-averaged temperature [K] in the plenum. The location of the graphite is similar to Figure 5.7. The graphite is visible in the lower part of each plot in a deep blue. See Figure 4.3 for original geometry.

The velocity average around the tip is affected by the extent of flow separation experienced by the flow exiting the channel - a gradual transition with a long tapered tip minimises local flow separation and turbulence while an abrupt transition due to a flat-top is more likely to lead to strong and persistent local vortices. The average velocity values in the plenum indicate the extent of the large recirculation vortices formed above the graphite, which
Table 5.3: Temporal and spatial averages of z-velocity around graphite tip.

<table>
<thead>
<tr>
<th>Case</th>
<th>Average velocity plenum</th>
<th>Average velocity tip</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Volumetric average</td>
<td>Volumetric average</td>
</tr>
<tr>
<td></td>
<td>(m s(^{-1}))</td>
<td>(m s(^{-1}))</td>
</tr>
<tr>
<td>30°</td>
<td>0.05119</td>
<td>0.06184</td>
</tr>
<tr>
<td>45°</td>
<td>0.05044</td>
<td>0.06277</td>
</tr>
<tr>
<td>60°</td>
<td>0.04983</td>
<td>0.06286</td>
</tr>
<tr>
<td>90° (flat)</td>
<td>0.04889</td>
<td>0.04889</td>
</tr>
</tbody>
</table>

Table 5.4: Velocity data near the tip of the stringer.

<table>
<thead>
<tr>
<th>Case</th>
<th>Time-averaged max. Value (ms(^{-1}))</th>
<th>Location (in.,in.,in.)</th>
<th>Time-averaged min. in plenum Value (ms(^{-1}))</th>
<th>Location (in.,in.,in.)</th>
<th>Time-averaged min. near tip Value (ms(^{-1}))</th>
<th>Location (in.,in.,in.)</th>
</tr>
</thead>
<tbody>
<tr>
<td>30°</td>
<td>0.40256</td>
<td>(0,-0.99,-0.37)</td>
<td>-0.03881</td>
<td>(0.02,0.04,5.37)</td>
<td>-0.02463</td>
<td>(0.45,-0.12,1)</td>
</tr>
<tr>
<td>45°</td>
<td>0.40267</td>
<td>(0.99,0,0.19)</td>
<td>-0.05520</td>
<td>(0.03,0.49,3.77)</td>
<td>-0.03530</td>
<td>(-0.78,0.87,1)</td>
</tr>
<tr>
<td>60°</td>
<td>0.40234</td>
<td>(0.99,0,0.55)</td>
<td>-0.04305</td>
<td>(-0.06,-0.05,3.84)</td>
<td>-0.01744</td>
<td>(-0.09,-0.37,1)</td>
</tr>
<tr>
<td>90° (flat)</td>
<td>0.40240</td>
<td>(0.99,0,1.01)</td>
<td>-0.04059</td>
<td>(0.09,-0.08,4.64)</td>
<td>-0.03095</td>
<td>(-0.06,0.138)</td>
</tr>
</tbody>
</table>

Figure 5.9: Trends seen in non-dimensional average volumetric (for salt) and surface (for graphite) temperatures in the plenum.

Entrap and heat the fuel salt, and the degree of mixing between the jets emerging from the channels and the salt in the plenum. The temperature averages of the graphite surface, the salt around tip, and the salt in the plenum are affected accordingly by the extent to which turbulence enhances mixing and heat transfer in these regions.

Starting with the 30° case, we found that the volumetric average velocity around the tip was the second lowest of the four cases (Table 5.3). The minimum z-velocity was the second highest of the four (Table 5.4). This suggests that
the long, tapered shape of the tip minimises flow separation and turbulence around the tip, and the salt slows down as it moves along the surface of the tip in a relatively laminar fashion after exiting the channel. This case also has the highest average velocity in the plenum, which when coupled with the largest (i.e. the least negative) minimum velocity value indicates that the turbulence in the plenum is low and the strength of the recirculation vortices in the plenum is relatively feeble. Due to the minimal flow separation around the tip, the jets from the channels emerge relatively intact and preserve their profile until they reach the outlet. This can also be observed in Figures 5.5 and 5.7. The slow, laminar flow explains why the graphite surface is the hottest of the four cases, and the volume of salt
around the tip is the second hottest of the four, due to the long residence time of the radioactive salt around the tip. However, the plenum is relatively cold because the hot jets from the channel are not mixing with the colder salt in the plenum, and with minimal recirculation and turbulence, heat transfer between the jets and the plenum salt is largely conduction based and hence rather poor.

Next we discuss the 45° case, which closely resembles the original Molten Salt Reactor Experiment (MSRE) stringer design (Figure 4.2). In contrast to the 30° case, the 45° case shows the most-negative minimum velocity values, both around the tip and the plenum (Table 5.4). Figures 5.7 and 5.8 demonstrate significant turbulence around the tip, and secondary vortices downstream from the tip. Figure 5.5 also shows the greatest amount of mixing between the hot jets from the channels and the cold plenum salt. This results in excellent heat transfer in the plenum from the jets to the salt, resulting in an overall colder plenum, which also translates into the graphite surface being cooler than the rest of the geometries. We posit that this stems from the tip being tapered enough to create significant local flow separation around the end of the channel, destabilising the emerging jets and creating lots of mixing. These less-stable jets, coupled with the relatively large size of the tip and secondary downstream vortices, also destabilise the larger recirculation vortices seen in the other cases that are likely to trap fuel salt where it heats up.

The 60° case and the flat-top case display many similarities as the geometry and the profile of the stringer-top in both cases is similar. However, the 60° case exhibits the largest average velocity around the tip, and the largest and least negative minimum velocity value around the tip. While the expectation is that the short, shallow tip is going to create flow separation from the jets and generate turbulence around the tip, the small size of the tip means that the small local vortices formed from flow separation mix easily and dissipate. Meanwhile, the larger recirculation vortex that is set up in the plenum is formed by separation from the jets near the outlet, and the separated layer flowing downward towards the tip. On approaching the tip, it finds a small, shallow obstacle that gradually channels the flow upwards again (Figure 5.7). In other words, the small size and taper of the tip sustains these recirculation vortices, seen on either side of the centre-line in Figure 5.7. These quasi-stable larger recirculation vortices are sweeping up and disrupting the smaller local flow separation eddies, explaining the high velocity average around the tip and the low turbulence observed in the figures. The figure also shows few secondary vortices in the plenum, and the average velocity in the plenum is the second lowest, confirming the presence of four strong primary recirculation vortices, one above each half channel, wherein the salt is trapped and continuously recirculating. This also explains why the volumetric average of the salt temperature is the highest of all four cases (Table 5.2), and the graphite tip surface is also relatively hot due to the trapped hot salt plus enhanced heat transfer due to turbulent local flow separation eddies (Figure 5.8).

The flat top case predictably has the lowest average velocity both near the tip of the stringer and in the plenum,
due to the abrupt flow separation encountered by the jets emerging from the half channel into the plenum (Table 5.7). The strong turbulence near the tip and the reflection of the recirculation vortices from the flat top as they flow down from the outlet also destabilises the jets further downstream, creating secondary quasi-stable vortices (Figure 5.7) that somewhat enhance mixing in the plenum. These result in the trapped salt heating up such that the average volumetric temperature is the second highest, but less than the 60° case which has more stable recirculation vortices and fewer secondary downstream vortices (Figure 5.7 and 5.8). The graphite surface, however, is hotter than the 60° case as there is greater turbulence in the flat top case, because there is no angled tip to minimise flow separation therefore the increased turbulence enhances heat transfer between the salt and the graphite.

### 5.2 Discussion

The results clearly demonstrate that recirculation vortices are formed in the upper plenum above the graphite stringer where the fuel salt is trapped in vortices for some time. This is similar to the observations made by Podila et al. [33]. However, this does not lead to any significant heating of the salt. The stringer tip size and shape influence the flow and temperature in the plenum of the Molten Salt Reactor Experiment (MSRE). However, the impact of varying the tip shape and size is small. The range of volumetric and surface average temperatures across the four cases is less than 3K. Therefore, while incorporating a stringer-tip similar to our 45° case would bring any MSRE simulation closer to the original geometry (Figure 4.2), neglecting the pyramid tip and approximating it with a flat top is unlikely to introduce significant inaccuracies in any Computational Fluid Dynamics (CFD) model.

Comparison of the flow around the four stringer geometries shows turbulence plays a small role at the relatively low Reynolds number of 1000 due to flow separation and salt recirculation in the upper plenum. Meshing this tip from a CAD model or deforming it on the fly is a non-trivial task, hence many analyses neglect this geometrical feature [85, 33]. Incorporating the effects of this tip could help improve the accuracy of MSRE thermal-hydraulic simulations, especially in the plenum. For instance, the recirculation zones we have seen were also present in the Reynolds-Averaged Navier Stokes (RANS)-based simulations conducted by Podila et. al [33]. Our models indicate that if they had incorporated the pyramid tip for each stringer's mesh, the recirculation they saw in the upper plenum could have been mitigated.

The analysis also illustrates the nuances introduced by variation in geometry. Minimising flow separation using the 30° tip or maximising turbulence using a flat top may not necessarily yield the best results. As the 45° case shows the best thermal characteristics in the plenum, it follows that for this particular geometry there is a certain sweet spot when it comes to tip size and apex angle that is ideal for using flow separation to minimise laminar flow as the jets exit the channel, for disrupting the larger recirculation vortices in the plenum, and for promoting
mixing of the jets in the plenum. Too little flow separation as in the 30° case minimises mixing and increases the
case, making the graphite too hot. On the other hand, as we approach a flat-top with the 60° and the 90° (flat) case, the flatter geometry makes it easier for the recirculation vortices to set up and remain stable despite flow separation at the end of the MSRE channel, because the recirculation vortex is much larger and stronger and a flatter tip does not disrupt it as much. These insights can be applied to any MSRE-like design as long as the operating conditions and geometry are not significantly different.

In considering the relevance of these results to other Molten Salt Reactors (MSRs), we posit that if the Reynolds number were higher, turbulence would improve mixing and heat transfer in the channel and the plenum and mitigate the temperature differences observed. Such operating conditions would also disrupt the quasi-stable recirculation vortices which trap and heat the molten salt. While the effects of varying the tip shape on the MSRE channel were not catastrophic, it may be possible that a larger core with bigger stringer-like structures could result in larger recirculation vortices in the plenum above said structures. The possibility of entrainment of significant quantities of fuel salt and its impact needs to be investigated in any larger variant of the MSRE.

This also indicates the need for modelling turbulence at relatively low Reynolds numbers wherever flow separation is likely to be significant, as neglecting the effects of turbulence in such geometries could affect the outcomes of thermal safety analyses in larger cores. At the very least, there is a need for local CFD models of specific areas of concern such as reactor plena using medium-fidelity RANS models. Development of high-fidelity multiphysics simulation strategies using fast, scalable, and low memory-footprint computational techniques that can leverage the next generation of high-performance computing machines will likely prove vital for performing these CFD simulations and aid the licensing of any new MSR design where salt entrainment and recirculation is a possibility.
Chapter 6

Conclusions

We simulated the flow of molten salt around a Molten Salt Reactor Experiment (MSRE) graphite stringer at standard MSRE operating conditions using the Large Eddy Simulation (LES) capabilities of Nek5000. In particular, we analysed the sensitivity of the flow to the shape of the pyramidal tip of the stringer, and its effects on the temperature of the graphite stringer and the molten salt in the plenum. To our knowledge, this is the first study that incorporates the pyramidal stringer tip and analyses its effects, and is also the first application of LES to the MSRE.

After briefly introducing the need for MSRs in Chapter 1, we discussed the theoretical background needed to understand these simulations in Chapter 2. In Chapter 3, we review state-of-the-art MSRE simulations and how flow in other geometries and reactor cores has revealed turbulent instabilities at relatively low Reynolds numbers. We point to the knowledge gap we are exploring, namely investigating the overall significance of the effects of flow separation and salt recirculation within the MSRE and the effect of different stringer tip configurations on the fuel salt and graphite temperature. We reviewed the MSRE reactor geometry and simulation parameters in Chapter 4.

Results from Chapter 5 indicate that perturbing the shape of the stringer tip does not lead to a sizeable increase in the maximum temperature observed in the MSRE channels. It affects the temperatures observed in the MSRE plenum over a range of less than 3 K. Therefore the pyramid tip may be neglected in the Computational Fluid Dynamics (CFD) simulations of the MSRE.

The pyramid shape with an apex half-angle of 45° performs the best as the shape of the tip maximises flow separation at the end of the channels and promotes local mixing, and the substantial tip coupled with the aforementioned flow separation disrupts the larger recirculation vortices in the plenum which have a tendency to trap the molten salt. As a result, the graphite surface is the coldest of the four cases, and the salt temperature in the plenum is also the lowest. The 30° tip has the hottest graphite surface, by 2 K, due to the laminar flow of the salt along the tip, increasing its residence time in the region around the tip. The salt in the plenum does not undergo significant mixing as the jets stay relatively intact, leaving the plenum salt relatively cold. The 60° and flat-top cases exhibit similarities in their thermal characteristics. The flatter tops readily sustain the large recirculation vortices in the plenum wherein the salt is trapped and heats up continuously, also transferring heat to the graphite surface. The 60° case displays more stable recirculation vortices due the shallow angled tip stabilising the rotational flow of the
vortices between the outlet and the tip, resulting in hotter salt in the plenum compared to the flat-top case. The larger, more stable recirculation vortices also suppress the smaller flow separation vortices near the tip, prevent efficient mixing of the salt across the tip and the plenum volume, and degrades heat transfer between the salt and the graphite, leaving the surface colder than the flat top case. The flat top case also has dominant recirculation vortices but these are more unstable and turbulent due to the abrupt reflection they encounter at the flat-top surface, leading to better mixing in the plenum and around the tip. The significant turbulence around the flat-top from local flow separation vortices improves heat transfer between the salt in the plenum and the graphite surface. This makes the salt colder but the graphite surface warmer than the 60° case.

Our results demonstrate that geometry-induced flow separation can create turbulence at low Reynolds numbers and these effects can alter the temperature of the fuel salt and structural material in a channel-type MSR. Within the MSRE, these effects are not substantial. These effects are likely to be more significant in a larger MSRE-like core, however. In such a reactor, similar but larger vortices could persist above bigger stringer-like structural materials and entrain a volume of salt greater than the amount seen in these MSRE recirculation zones. The ideal stringer geometry disrupts the flow at the end of the channel and inhibits the entrainment of molten salt in the plenum, leading to lower temperatures. For such larger variants of the MSRE, these geometry-specific effects need to be analysed with accurate meshing of structural features and by performing medium- to high-fidelity turbulence modelling using Reynolds-Averaged Navier Stokes (RANS) or LES, especially for regions such as plena.

Natural extensions of this project would involve simulating the salt flow in the entire plenum. This salt behaviour cannot be adequately modelled using our mesh with periodic boundary conditions. Using a wedge-like section that extends radially from the centre of the plenum to its periphery, representing just an eighth or a quarter of the plenum, would lead to a more accurate picture of the flow in the plenum. The domed shape of the MSRE plenum will create a radially inward and upward current towards the outlet that will disrupt many of the quasi-stable vortices formed above multiple stringers. The significance of the effects of any recirculation zones that persist despite the aggregate flow in the plenum must be assessed. A comparison of RANS and LES approaches would also be instructive in determining the level of detail required for modelling turbulence in such Molten Salt Reactors (MSRs). As discussed in Chapter 3, turbulent oscillations can be observed over a range of Reynolds numbers in multiple geometries, and the ideal Reynolds number that mitigates these salt recirculation zones must be determined using high-fidelity CFD simulations. Lastly, coupling these thermal-hydraulic simulations with neutronics while also tracking delayed neutron precursors will increase the accuracy of MSR simulations. In particular, it will help determine whether these recirculation vortices trap enough precursors to significantly alter the neutron flux and hence the source term, which could lead to interesting dynamic behaviour.
Appendices
Appendix A

Filtered Conservation Equations

For our illustrative example, we consider *homogeneous filters* [114], which are linear, symmetric functions that do not affect constants in their filtering operation. They allow filtering operations and spatial derivatives to commute, reducing the number of filtered terms in this example [35, 44, 114]. Using our definition of filtered velocity (Equation 2.42) in the incompressible Navier Stokes equations (Equation 2.21), we can obtain the following large eddy simulation equations.

**Conservation of Mass**

\[
\left( \frac{\partial U_i}{\partial x_i} \right) = \frac{\partial \overline{U}_i}{\partial x_i} = 0 \tag{A.1}
\]

\[
\frac{\partial u'_i}{\partial x_i} = \frac{\partial}{\partial x_i} (U_i - \overline{U}_i) = 0 \tag{A.2}
\]

\[
\overline{U}_i = \text{filtered velocity along the } i \text{ direction} \tag{A.6}
\]

\[
u'_i = \text{sub-grid scale velocity along the } i \text{ direction} \tag{A.5}
\]

\[
U_i = \text{unfiltered velocity along the } i \text{ direction} \tag{A.4}
\]

These equations demonstrate that the filtered field (Equation A.2) and the residual field (Equation A.3) are both divergence-free.
Conservation of Momentum

The filtered momentum equation is

\[
\frac{\partial U_j}{\partial t} + \frac{\partial U_i U_j}{\partial x_i} = \nu \frac{\partial^2 U_j}{\partial x_i \partial x_i} - \frac{1}{\rho} \frac{\partial \bar{p}'}{\partial x_j}
\]  

(A.8)

where

\[
p' = \text{filtered pressure} \quad \text{(A.9)}
\]

\[
\nu = \text{kinematic viscosity. (A.10)}
\]

To further expand the non-linear convective term \(U_i U_j\), we utilise the Reynolds stress tensor

\[
\tau^R_{ij} = \overline{U_i U_j} - \overline{U_i} \overline{U_j}
\]  

(A.11)

and the anisotropic residual stress or sub-grid scale tensor

\[
\tau'_{ij} = \tau^R_{ij} - \frac{2}{3} k_r \delta_{ij}
\]  

(A.12)

where

\[
k_r = \frac{1}{2} \tau^R_{ii} = \text{residual kinetic energy} \quad \text{(A.13)}
\]

to expand \(\overline{U_i U_j}\)

\[
\overline{U_i U_j} = \overline{U_i} \overline{U_j} + \tau^R_{ij} = \overline{U_i} \overline{U_j} + \tau'_{ij} + \frac{2}{3} k_r \delta_{ij}.
\]  

(A.14)

Substituting the above result (Equation A.14) into equation A.8, we get

\[
\frac{\overline{D U_j}}{\overline{D t}} = \nu \frac{\partial^2 \overline{U_j}}{\partial x_i \partial x_i} - \frac{\partial \tau'_{ij}}{\partial x_i} - \frac{1}{\rho} \frac{\partial \bar{p}'}{\partial x_j}
\]  

(A.15)

where

\[
\overline{p} = p' + \frac{2}{3} \rho k_r = \text{modified filtered pressure} \quad \text{(A.16)}
\]

\[
\frac{\overline{D}}{\overline{D t}} = \frac{\partial}{\partial t} + \overline{U} \cdot \nabla = \text{filtered velocity-based material derivative. (A.17)}
\]
Here, $\bar{U}, \bar{p}$, and $\tau_{ij}$ are random, 3D, and time-dependent [35]. To simplify this problem in order to avoid computationally intensive integration for the above unsteady 3D velocity-pressure equation (Equation A.15), it is common practice to decouple the velocity and pressure solves (see Section 2.3).

The anisotropic stress tensor is represented by [35]

$$\tau_{ij}^R = \mathcal{L}_{ij}^o + \mathcal{C}_{ij}^o + \mathcal{R}_{ij}^o$$  \hspace{1cm} (A.18)

where

$$\mathcal{L}_{ij}^o = \bar{U}_i \bar{U}_j - \bar{\bar{U}}_i \bar{\bar{U}}_j = \text{Leonard stresses}$$  \hspace{1cm} (A.19)

$$\mathcal{C}_{ij}^o = \bar{U}_i u'_j - \bar{u}'_i \bar{U}_j - \bar{\bar{U}}_i \bar{\bar{U}}'_j + \bar{\bar{U}}'_i \bar{U}_j = \text{Cross stresses}$$  \hspace{1cm} (A.20)

$$\mathcal{R}_{ij}^o = \bar{u}'_i \bar{u}'_j - \bar{\bar{u}}'_i \bar{\bar{u}}'_j = \text{SGS Reynolds stresses.}$$  \hspace{1cm} (A.21)

For a sharp spectral filter, the anisotropic tensor for wave-number $K$ may be simplified to [35]

$$\tau^K_{ij} = \mathcal{R}_{ij}^o + \mathcal{C}_{ij}^o$$  \hspace{1cm} (A.22)

$$= \bar{u}_i \bar{U}_j + \bar{u}_j \bar{U}_i + \bar{\bar{u}}'_i \bar{\bar{u}}'_j.$$  \hspace{1cm} (A.23)

This formulates each component of the tensor in terms of filtered quantities, represented exactly by the filtered/re-solved modes with $K < K_c$.

However, even this simplified form is computationally expensive to calculate for multiple time steps. These tensor forms must be approximated to obtain an inexpensive expression for the sub-grid scale tensor $\tau^K_{ij}$, and to obtain closure for the filtered Navier-Stokes equations (Equation A.15). This has motivated the creation of several sub-grid scale models [44, 114] like the Smagorinsky Model [43].

**Conservation of Energy**

The filtered conservation of energy equations represent the transfer of kinetic energy between the filtered and residual velocity fields. The filtered kinetic energy is given by

$$\bar{E} = \frac{1}{2} \bar{U} \cdot \bar{U} = E_f + k_r$$  \hspace{1cm} (A.24)
where

\[ E_f = \frac{1}{2} \bar{U} \cdot \bar{U} = \text{filtered velocity field's kinetic energy} \] (A.25)

\[ k_r = \frac{1}{2} \bar{U} \cdot \bar{U} - \frac{1}{2} \bar{U} \cdot \bar{U} = \frac{1}{2} \bar{\tau}^R_{ij} = \text{is residual kinetic energy.} \] (A.26)

By multiplying the momentum equation A.15 with \( \bar{U}_j \), we get the energy equation

\[ \frac{\partial E_f}{\partial t} - \frac{\partial}{\partial x_i} \bar{U}j \left( 2v \bar{\delta}_{ij} - \frac{\bar{p}}{\rho} \delta_{ij} \right) = -\epsilon_f - \mathcal{P}_r \] (A.27)

where

\[ \epsilon_f = 2v \bar{S}_{ij} \bar{S}_{ij} = \text{viscous dissipation from filtered velocity} \] (A.28)

\[ \mathcal{P}_r = -\tau^R_{ij} \bar{S}_{ij} = \text{production/source term for residual kinetic energy} \] (A.29)

\[ \bar{S}_{ij} = \frac{1}{2} \left( \frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) = \text{filtered rate-of-strain tensor.} \] (A.30)

In most high Re flow LES where \( \Delta >> \eta \), the \( \epsilon_f \) term is negligible, and so is \( k_r \). Physically, \( \mathcal{P}_r \) is responsible for transferring kinetic energy from filtered to residual motions. Overall, energy is transferred from large scale to small scale eddies (i.e. \( \mathcal{P}_r > 0 \), but locally, energy backscatter from small scale to large scale eddies may occur, locally i.e. \( \mathcal{P}_r < 0 \) is possible. Therefore it appears as a negative sink term in the filtered kinetic energy \( \bar{E} \) equations, but as a positive source term if the equation is framed in terms of the local residual kinetic energy \( k_r \).
Appendix B

Spectral tensor contraction implementation

Consider a 2D operator $C$ formed as a tensor product of $N \times N$ 1D operators $A$ and $B$

$$C = A \otimes B$$ (B.1)

applied to a vector $u$, i.e. $Cu$, which is typical in iterative solvers. Using the Kronecker product's mixed-product property\[37]:

$$PQ \otimes RS = (P \otimes R)(Q \otimes S)$$ (B.2)

we can express the action of the 2D operator as:

$$Cu = (A \otimes B)u$$ (B.3)

$$= (AI) \otimes (BI)u = (A \otimes I)(I \otimes B)u$$ (B.4)

where

$$I = N \times N \text{ identity matrix}$$ (B.5)

Using the definition of the Kronecker product from equation 2.86, we can expand the first operation of the above equation, i.e. $W = (I \otimes B)u$ as

$$w_{ij} = \sum_{k=1}^{N} b_{ik} u_{kj}$$ (B.6)

$$W = BU$$ (B.7)

where

$$U = \text{vector } u \text{ reshaped into an } N \times N \text{ matrix}$$ (B.8)
Similarly, we find that the application of the second operator, \((A \otimes I)\), can be expressed as

\[
  v_{ij} = \sum_{l=1}^{N} a_{il} w_{jl} \quad \text{(B.9)}
\]

\[
  = \sum_{l=1}^{N} w_{jl} a_{ij}^T \quad \text{(B.10)}
\]

\[
  V = WA^T \quad \text{(B.11)}
\]

Substituting these results into equation B.4, we get:

\[
  Cu = (A \otimes B)u = BU A^T \quad \text{(B.12)}
\]

While the original tensor product evaluation (equation B.4) costs \(2N^4\) operations, when reduced to matrix-matrix products as above, the operations cost \(4N^3\). A similar form exists for 3D operators. An operation of the form

\[
  Du = (A \otimes B \otimes C) = (A \otimes I \otimes I)(I \otimes B \otimes I)(I \otimes I \otimes C)u \quad \text{(B.13)}
\]

can be expressed as a sequence of matrix-matrix products in three steps. The first operation \((I \otimes I \otimes C)u\) becomes:

\[
  W = (I \otimes I \otimes C)u = CU \quad \text{(B.14)}
\]

where

\[
  U = \text{vector } u \text{ reshaped into an } N \times N^2 \text{ matrix} \quad \text{(B.15)}
\]

After this step, \(W\) can be reshaped into an \(N \times N \times N\) brick, or a 3D array expressed as a sequence of \(N\) matrices of size \((N \times N)\). The second operation \((I \otimes B \otimes I)W\) can be expressed as:

\[
  V_i = BW_i \quad \text{(B.16)}
\]

where

\[
  W_i = i^{th} N \times N \text{ array of } W \quad \text{(B.17)}
\]
The 3D \( V \) array can now be reshaped into an \( N^2 \times N \) matrix, making the final operation \((A \otimes I \otimes I)V:\)

\[
Y = VA^T
\]
Appendix C

Nek5000 mesh deformation code

The following code was inserted in Nek5000's userdat2 function to modify the flat-top mesh to the three different configurations mentioned in the thesis.

```
include 'SIZE'
include 'TOTAL'

common /comprams/ dh,dhsi,zc1,zc2,zc3,uav
real height, theta
real xmin, xmax, ymin, ymax, zmin, zmax

ntot = nx1*ny1*nz1*nelt

theta = pi/4.0
_c = cos(theta)
s = sin(theta)

do i=1,ntot
   x=xm1(i,1,1,1)
y=ym1(i,1,1,1)
xm1(i,1,1,1) = c*x - s*y
ym1(i,1,1,1) = s*x + c*y
endo

call domain_size(xmin,xmax,ymin,ymax,zmin,zmax)
```
height = 1.0 ! height = sqrt(3.0) for 30 degrees, 1 for 45 degrees, 1/sqrt(3.0)

do i=1,ntot
    x=abs(xm1(i,1,1,1)/xmax)
    y=abs(ym1(i,1,1,1)/ymax)
    z=z(m1(i,1,1,1))
    Lg=63.0
    Lp=7.0
    zt=1.0 ! tip location
    if (z.gt.zt) then
        zm1(i,1,1,1) = zm1(i,1,1,1)-height*(x+y)*(zmax-z)/Lp
    else
        zm1(i,1,1,1) = zm1(i,1,1,1)-height*(x+y)*(z-zmin)/Lg
    endif
endo

endo

do i=1,ntot
    x=xm1(i,1,1,1)
    y=ym1(i,1,1,1)
    xm1(i,1,1,1) = c*x + s*y
    ym1(i,1,1,1) = -s*x + c*y
endo
References


