University of Southern Queensland

Faculty of Engineering and Built Environment

DEVELOPMENT OF ADVANCED TURBULENT COMBUSTION MODELS

Dissertation submitted by

Matt V. Pichlis

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ABSTRACT

Due to the increasing concern of energy security and the environmental issues related to energy production it is the responsibility of engineers to develop improved systems. Systems are required that are more efficient and therefore reduce pollution, while still being economical. This can be achieved through the development of new alternative energy sources or by improving existing sources such as combustion systems.

An effective way of analysing and improving combustion systems is through the use of simulations. This is a much cheaper and easier method than using test models. However because combustion is so complex the most accurate simulations are only able to calculate for very small and simple volumes ($<$ $1\ cm^3$). Therefore models are used to simulate for a realistic size combustion chamber.

The relatively new Multiple Mapping Conditioning (MMC) model has been developed and validated for certain cases. It is derived from the Conditional Moment Closure (CMC) model, probability density function methods and combined with a Mapping Closure to utilize the benefits of each method. This project has aimed to further develop the use of the MMC model for the application to a partially stirred reactor (PaSR).

The model has been developed by updating the chemical kinetics to a more simplistic approach. Cantera toolbox for MATLAB was used as it is capable of performing the reaction equations more simplistically than the previous methods. The boundary conditions of the model were also developed in order to resolve the problems that the model encountered previously.

Simulations were performed to investigate the accuracy and efficiency of the model over a range of conditions and comparisons with existing literature and other models are drawn. Temperature and mixing profiles are generated to understand the behaviour of the combustion system. The simulations provided results that were in agreement with the existing literature and expected behaviour. This suggests that the MMC model is viable for the application to a partially stirred reactor.

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Certification of Dissertation

I certify that the ideas, designs and experimental work, results, analyses and conclusions set out in this dissertation are entirely my own effort, except where otherwise indicated and acknowledged.

I further certify that the work is original and has not been previously submitted for assessment in any other course or institution, except where specifically stated.

M. Pichlis

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1 BACKGROUND

1.1 INTRODUCTION

With finite supplies, and increasing prices of fossil fuels such as oil and coal it is important that these resources are used as effectively as possible. Fossil fuels are commonly used in the combustion leading to power generation. Combustion is the chemical reaction between the fuel and an oxidiser in which energy is released. This energy is generally in the form of heat which can then be harnessed and converted to electrical energy. This is a common process in power stations where a furnace heats a boiler to create steam which allows the production of electricity. To ensure highest amount of energy possible is being gained, a deeper understanding of this combustion process

is required. However because of the nature of combustion, it is difficult or impossible to gain real life physical data of some aspects. This demonstrates the importance of combustion modelling.

Combustion modelling provides an insight into the details of combustion such as the mixing of fluid particles within the reaction zone and the chemical species that will be output. By being able to understand all aspects of the combustion process the system can be analysed and improved. Improving the system can mean increasing efficiency so that less fuel is needed to produce the same energy output, changing the concentrations of the exhaust species to make a healthier and more environmentally friendly system, or to increase the life of a system. These are all beneficial outcomes that will reduce costs and save money. Combustion modelling allows a more complete understanding of a system that can ultimately lead to changes being made and resulting in more efficient and environmentally friendly combustion.

There is a wide range of combustion models with varying accuracy and ease of use. Modelling is used as a representative form of the combustion system whereas more accurate methods such as direct numerical simulations solve the problem exactly. Modelling is required as solving exactly is computationally intensive and therefore only possible for very small volumes. Models aim to replicate the mixing and results using more simplistic methods applied to realistic sized problems. Some common model types include probability density function models (PDF) and the conditional moment closure model (CMC) that are both used in the formulation of the multiple mapping conditioning model (MMC). Different model types are used depending on the requirements and are generally developed for the application to a particular situation. This includes different reactor types that can then be used together to represent a realistic combustion system.

The focus of this project lies on the application of the MMC model to a partially stirred reactor (PaSR). Current literature available on this topic was reviewed and it was found that there was plenty of literature based on the

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older turbulent combustion models such as the probability density function based methods however the more recent models were lacking in relevant information. For the case of multiple mapping conditioning applied to a partially stirred reactor the most relevant sources were Wandel's thesis "Development of Multiple Mapping Conditioning (MMC) for Application to Turbulent Combustion" (2005) and the paper by Sundaram "Prediction of extinction modes for turbulent premixed combustion with an MMC-Partially Stirred Reactor" (2013). These sources did not successfully apply the MMC to a PaSR to obtain results for temperature prediction or species emissions and therefore there is a need for further development in this area.

1.2 AIMS AND OBJECTIVES

The aims and objectives of this project as detailed in the project specification are:

1. Research and study the turbulent combustion model, 'Multiple Mapping Conditioning' (MMC)
2. Investigate the case of a 'Partially Stirred Reactor' (PaSR)
3. Determine appropriate boundary conditions for MMC applied to PaSR
4. Simulate for a wide range of conditions to verify the model
5. Investigate the efficiency and accuracy of different forms of MMC

1.3 OFFER OF THE PROJECT

This project was offered by the faculty under the supervision of Dr. Andrew Wandel. Andrew is a leading researcher in the field of combustion modelling and this project focusses on the continuation of one of his previous projects. In Andrew's thesis, 'Development of Multiple Mapping Conditioning

(MMC) for Application to Turbulent Combustion' the Multiple Mapping Conditioning model was applied to a partially stirred reactor (Wandel 2005). At the time it was deemed not suitable, the aim of this project is to further develop this model and try to prove its effectiveness for the partially stirred reactor.

2 LITERATURE REVIEW

The literature available for combustion modelling in general is very broad due to the amount of models and possible cases that they can be applied to. However when a specific model and case are detailed the amount of literature available is dramatically reduced. For the case of the Multiple Mapping Conditioning model applied to a Partially Stirred reactor there is very limited previous work. The main source for this project being 'Development of Multiple Mapping Conditioning (MMC) for Application to Turbulent Combustion' by Wandel, where the code was created that is to be developed by this project (2005). The limited literature highlights the possibility for this model to be further developed and proven as a viable model for the specific application.

2.1 COMBUSTION BACKGROUND

Combustion is one of the most common forms of energy production. Combustion, or burning is an exothermic sequence of chemical reactions between a fuel and an oxidiser known as the reactants. The conversion of the chemical species results in the production of heat, energy and a number of chemical species known as the products. Combustion is used in many engineering applications such as internal combustion engines and furnaces or boilers used in power stations. Combustion can take different forms depending if the reactants are mixed together before entering the combustion zone (premixed) or if the fuel and oxidiser enter the combustion zone separately (non premixed). The form also depends on the method of ignition with some types requiring an external spark whereas other forms can auto ignite due to temperature increase under pressure.

The combustion process can also be defined as laminar or turbulent. This is depending on the state of the fluid as it flows through the combustion area and can be determined by finding the Reynolds number. Turbulent combustion is more prevalent in things such as combustion engines where the mass flow rate is high and the combustion process is very rapid. Laminar combustion can be seen in situations such as burning a candle in a quiescent environment.

The process of combustion depends heavily on the mixture fraction of the reactants. The mixture fraction is defined;

$$Z = \frac{Y_F}{Y_F + Y_O} \tag{2.1}$$

Where $'Y_F'$ is the mass fraction of fuel and $'Y_O'$ is the mass fraction of oxidiser. The mixture fraction will result in a value between one and zero with one meaning the fluid is complete fuel and zero is complete oxidiser. At a specific mixture fraction the fuel and oxidiser will be completely consumed throughout the reaction process. This is known as the stoichiometric mixture fraction. The chemical equation for the stoichiometric combustion of hydrogen and air is as below:

$$H_2 + \frac{1}{2}(O_2 + 3.76N_2) \rightarrow H_2O + 1.88N_2 \tag{2.2}$$
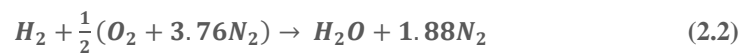
In most cases stoichiometric combustion is not used, instead the combustion will be made 'lean' by adding more oxidiser than required for complete combustion. This is often done to ensure that all the fuel is completely burnt as unburnt fuel can contain harmful products. The disadvantage of running a lean combustion system is that by decreasing the mixture fraction the chances of extinction or failure to combust are increased. In some cases to ensure that the flame does not extinguish an excess of fuel will be used causing a rich mixture. This is not effective as it results in unburnt fuel, therefore the combustion is not obtaining the maximum amount of energy possible and the efficiency of the system is decreased. The unburnt fuel also causes an increase in potentially harmful exhaust products.

2.2 TURBULENT COMBUSTION MODELLING

2.2.1 BENEFITS OF COMBUSTION MODELLING

Combustion Modelling proves an important tool for understanding and implementing combustion systems in real life applications. Because of the nature of combustion it is difficult to obtain experimental data and therefore models are relied on to provide an insight. By using combustion models it is possible to develop a greater understanding of a combustion system and

factors such as temperature, exhaust emissions and efficiency can be predicted. This information is vitally important in the design of new combustion systems as well as improving and maintaining current systems.

The main priority of improving a combustion system is to improve the efficiency. Improving the efficiency of the system will reduce fuel usage and running costs. In Australia the average price for unleaded fuel has increased from approximately 126 cents per litre in 2009 to about 150 cents per litre (AIP 2014). This demonstrates that it is becoming increasingly important to ensure that any combustion system uses the least amount of fuel as possible. However by reducing the amount of fuel used during the combustion process there are also some negative effects. In most combustion systems a rich mixture is more likely to be used to ensure that there will be no extinction of the flame and constant combustion will be maintained. In order to maximise efficiency a mixture fraction needs to be determined that will ensure no extinction while also using the least amount of fuel as possible.

Another major benefit of combustion modelling would be to analyse and predict the exhaust products. There has been an increasing strictness on emissions with schemes such as the Emissions trading scheme possible being introduced in Australia and in Europe with the EU emissions trading system (EC 2014). The protection of people's health and prevention of damage to the environment are paramount. The combustion of gasoline as used in most cars, leads to the exhaust of harmful products such as carbon monoxide (CO) and nitrogen oxides (NOx). Carbon Monoxide is poisonous to humans and can cause nausea or even death (DEH 2005). Exhaust gases are also a contributor to air pollution and the greenhouse effect which has led to the introduction of catalytic converters in Australian cars since 1986 (DIT 2011). The converters remove unburnt fuel and toxic pollutants from the exhaust. Therefore it is vitally important to reduce the concentration of harmful exhaust products and by using combustion modelling it is possible to predict these concentrations and attempt to improve the system.

2.2.2 REACTORS

Models are generally made to represent a reactor. The reactor is the space in which the combustion reaction occurs. There are several different types of reactors and by modelling each one separately they can then be combined to represent a complete system.

Some common reactor types include:

- Perfectly Stirred Reactor (PSR)
- Partially Stirred Reactor (PaSR)
- Plug Flow Reactor (PFR)
- Partially Stirred Plug Flow Reactor (PaSPFR)

A perfectly stirred reactor has an inflow rate equal to its outflow rate and a high rate of mixing. The high rate of mixing causes a uniform dispersion of fuel and oxidiser throughout the entire reactor. Therefore if a sample was taken from the outflow of the reactor it should match the concentrations within the reactor. Similar to a PSR, a partially stirred reactor has an equal inflow and outflow, however the rate of mixing or residence time is lower meaning that a uniform dispersion is not achieved. Therefore within the reactor there will be parts where the concentration is different to other parts of the reactor. For combustion this means that some areas could possibly have a concentration that does not allow complete combustion. Another common type of reactor is the plug flow reactor. A plug flow reactor is generally like a pipe where the reactants are introduced at a constant rate. The reactions occur as the fluid flows through the pipe. A normal plug flow reactor will achieve a uniform dispersion by the time it reaches the outflow whereas a partially stirred plug flow reactor will not.

2.2.3 TYPES OF COMBUSTION MODELS

There are several different types of combustion models that have been developed. These models range greatly in accuracy, ease of use and the situations that they can be applied to. Some simulations such as Direct Numerical simulations (DNS) are used for high accuracy however they can only be applied to very small volumes. DNS works by directly solving the Navier-Stokes equation for each node in a meshed control volume. This provides highly accurate results however at present computers are incapable of solving these calculations for engineering scale flows. Therefore DNS models are used mainly for comparison with other models as a test of accuracy.

Other models such as the Multiple Mapping Conditioning model simulate for an entire reactor. There are several types of reactors and models are developed for each type independently and then can be used together to represent a system. The models will allow for the flow rate of fluid particles into and out of the reactor as well as modelling all the mixing and chemical reactions that occur within. Most of these models are based on the probability density function. This is because turbulence is a random process and therefore exact replication is impossible. The MMC model is developed using a combination of the Probability Density Function Model (PDF) and the Conditional Moment Closure Model (CMC). By using a combination of these models some of the flaws are eliminated to try and produce a more accurate result. Some of the other models that are mentioned in this project include those used by in the paper by Ren and Pope (2004). The models used are:

- Interaction by Exchange with Mean (IEM) model (Dopazo & O'Brien 1974; Villermaux & Devillon 1972)
- Modified Curl (MC) model (Janicka, Kolbe & Kollman 1979)
- Euclidean Minimum Spanning Tree (EMST) model (Subramaniam & Pope 1998)

These models are used as a comparison for the MMC model applied to a partially stirred reactor. They are all pdf based methods and due to different mixing methods will result in a varied accuracy.

2.2.4 DIRECT NUMERICAL SIMULATIONS

Direct Numerical Simulations provide the most accurate form of combustion simulation. DNS works by creating a mesh for a given control volume and then solving the Navier-Stokes equation for each node within the mesh. The Navier-Stokes equation is derived from the conservation of momentum and defines a fluids flow. For accurate results the mesh used needs to very small, therefore the Navier-Stokes equation must be solved many time just to model a small control volume. This method is very computationally demanding and therefore there are limitations on the volume that can be modelled. Using modern computers a simulation that models a $1 \ mm^3$ volume can take days to complete. This means that DNS is not suitable for modelling fluid flows large enough to be applicable to most engineering applications. Therefore other models such as MMC are used when a larger scale system needs to be analysed. However because of the accuracy and the amount of data that DNS is able to record it is useful as a comparison for these other models.

2.2.5 PROBABILITY DENSITY FUNCTION MODELS

Due to DNS being unusable with the current computational power other methods are used to model turbulent combustion. Because turbulence is random the slightest change in the environmental conditions causes the process to be altered. Therefore because the exact conditions cannot be known statistical techniques are used to define the turbulence.

Let φ be a random variable and ψ is its sample space variable. If ψ is an axis of space that allows any value and φ is a variable that has a certain probability of taking a particular value of ψ-space. By determining this probability for each point in ψ-space a probability distribution can be defined. For many turbulent flows this distribution resembles the Gaussian or normal distribution for velocity. By averaging the probability density function the fluctuation can be determined as the deviation from the mean. Probability density function modelling forms the basis of the Multiple Mapping Conditioning model.

There have been a few cases of a pdf based model being applied to a partially stirred reactor. The paper by Ren and Pope (2004) is used throughout this project as a comparison for results. It demonstrates three different pdf models applied to the partially stirred reactor and the results are compared to test the performance of each model. The three models tested were the interaction by exchange with the mean (IEM) model (Dopazo & O'Brien 1974; Villermaux & Devillon 1972), modified curl (MC) model (Janicka, Kolbe & Kollman 1979) and the Euclidean minimum spanning tree (EMST) model (Subramaniam & Pope 1998). The conditional mean scalar dissipation implied by each model was deduced analytically or numerically but it was shown not to have the same significance as in other models such as conditional moment closure (CMC).

The IEM model is one of the simplest mixing models. It defines the mixing by using an exponential decay to the mean. This is not very accurate as it does not allow for any interaction between particles, however it has been proven useful for some cases (Pope 2000). The MC mixing model uses a different approach in that mixing occurs between pairs of particles. The pairs are determined using their probability and when mixed together both particles are given the same values depending on their old values. The disadvantage of this model is that the particle pairs can be made from anywhere throughout the scalar space. This means that particles from a parcel of fluid that is purely fuel could be mixed with other particles from anywhere within the reactor.

This does not resemble real life mixing as these particles would have no immediate interaction with the oxidiser. The EMST model is regarded as the most accurate method tested in this case. EMST mixing work by linking particles together for mixing. The links are dependent on the particles location in space and are made between particles closest together. The disadvantages of this is that because the links are made only between the particles closest together it does not allow for general mixing and causes an inaccuracy due to the locality of mixing.

Another comparison of some pdf based turbulent combustion models applied to a PaSR was performed by Orbegoso and Figuieira (2009). The models considered in this comparison were the Interaction by Exchange with the Mean, the extended IEM, Langevin and extended Langevin models. The models were compared showing that when mixing is fast and reaction is intense the different models lead to similar results. However when mixing is slow some differences are observed.

There are also a number of other pdf models that have been developed for a partially stirred reactor. However because of the varied conditions that are set for each it is difficult to make a direct comparison of results. Also because most models use pdf methods there is a broad spectrum that would need to be analysed. Therefore more specific MMC related models should be analysed for comparisons.

2.2.6 CONDITIONAL MOMENT CLOSURE

The Conditional Moment Closure (CMC) model is a more recent method of modelling turbulent reactive flows and it is used in the derivation of the MMC model. Conditional averaging is used where variables are conditioned on the sample space variable. Generally for non-premixed combustion the sample space variable is based on mixture fraction. By conditioning upon the sample

variable the quantities do not need to be modelled with respect to their spatial coordinates and therefore the number of independent variables is reduced. This is desirable as it makes the CMC model easier to use and from the mixture fraction probability distribution function, values for temperature and mass fractions can be estimated.

The verification and development of CMC methods for the prediction of turbulent reactive flows has been done by Klimenko and Bilger (1999). The paper details the different methods for the derivation of the CMC equation and simplifications that can be made for certain cases. The CMC predictions are compared with experimental results and direct numerical simulations to validate the method. A review is also made into the progress of the application of the CMC to problems involving multiple conditioning, differential diffusion, sprays and premixed combustion.

The paper by Kronenburg, Bilger and Kent (1998) was written in order to validate the second-order conditional moment closure for a turbulent flame. A system was modelled and then verified by comparison with experimental data. It was found that the model made excellent predictions of the output nitric oxide levels and in validated the model as suitable.

The CMC model has been applied to the partially stirred reactor by Mobini and Bilger (2009). For the paper titled 'Parametric study of the Incompletely Stirred Reactor modelling' a CMC model was formulated and applied to the PaSR. Some conclusions were determined relating the mixture fraction to the formation of nitric oxide that supported the validity of the model.

2.3 MMC MODEL

The focus of this project lies on the 'Multiple Mapping Conditioning' model, or MMC. The MMC model is a relatively new model for turbulent combustion modelling. It has been developed and verified by Klimenko and Pope in the paper 'A model for turbulent reactive flows based on multiple mapping conditioning'(2003). The validity of the model was demonstrated using a comparison with direct numerical simulations for the three-stream mixing problem.

MMC is derived from a combination of probability density function methods as well as the Conditional Moment Closure model. Aspects from both methods are used to take the advantages of each and try to eliminate any disadvantages. Generally pdf models provide the best results as they completely account for the fluctuations of the mass fraction of every species present during the reaction. This results in a complex calculation that can be difficult to solve as even simple systems with few input species can create many product species throughout the reaction. To simplify the model the species that are present in higher concentrations or deemed important (major species) can be modelled completely while the remaining species (minor species) are solved by conditionally averaging them on the major species. The Conditional Moment Closure uses this method of treating the species differently depending on their importance however because there is only one conditioning variable there are some fluctuations that cannot be appropriately modelled. MMC uses the benefits of pdf modelling for the major species and CMC for the minor species. A closure model is also required for any pdf model and for MMC mapping closure is used so that the dimensional scalar space is mapped onto a dimensional reference space. The MMC model satisfies all the properties of turbulent mixing including the localness or interaction, boundedness, independence of scalars and transition of scalar pdf to Gaussian in shape.

2.3.1 REFERENCE VARIABLE

The MMC model utilizes a reference variable to represent space in which the mixing can be analysed. The reference space is chosen to simulate for properties of turbulence that effect combustion such as mixture fraction, velocity components and dissipation.

The reference space is used to describe the transport of a quantity through the physical space of that quantity. The values of the reference space have a presumed probability and then mapping functions are determined that map the reference space to a space with the same probability as the probability of the physical space (Vogiatzaki 2009).

An example of the use of the reference space is in the difference between the EMST model and the MMC model. EMST determines localness directly from the composition space whereas MMC uses the reference variables to determine the localness. The disadvantage of the EMST model is that it does not allow for general mixing and causes an inaccuracy due to the locality of mixing. Using the reference space to determine locality, mixing can occur within a given range of that space.

2.3.2 DETERMINISTIC AND STOCHASTIC FORMULATION

The MMC model has been independently formulated using two different mathematical models, the deterministic model and the stochastic model. Deterministic models define every set of variable states from a given set of parameters and the previous states of those variables. This means that the model will produce the exact same results for a given set of initial conditions.

Stochastic models use a randomness where the variable states are not defined by given values but instead by probability distributions.

The deterministic formulation was proven viable by Klimenko and Pope (2003) by comparison with DNS for the three stream mixing problem. An equivalent stochastic formulation was presented as well. The stochastic formulation is expected to be more computationally efficient for multidimensional spaces.

Wandel (2005) made a comparison of the two formulations by creating a homogenous code for each method. The differences between the methods and strengths of each were outlined. It was found that the deterministic methods were better than the stochastic methods when the dimensionality of the reference space was small (i.e. one or two). If the dimensionality is larger the deterministic formulation is limited by its computational requirements and the stochastic formulation is preferred. The deterministic model also makes data available at almost continuous sampling whereas the stochastic method is very discrete. The stochastic model allows the time step to be changed to increase accuracy without greatly increasing the computational requirements. To increase accuracy with the deterministic formulation more data points would be required. It was concluded that the deterministic model is more intensive and requires more computational time, therefore best used with a small dimensionality of the reference space.

Vogiatzaki investigated the two formulations for application to turbulent reacting jets (2009). It was found that the deterministic methods predictions of reactive species and temperature were in good agreement with the experimental data. The stochastic method demonstrated potential in predicting the scattering around the conditional means however some discrepancies were noted. Vogiatzaki was also in agreement with the observations made by Wandel in that the stochastic method is preferred when dealing with spaces of large dimensions.

2.3.3 VERIFICATION OF THE MODEL

The MMC method has been verified by comparing it with other methods such as direct numerical simulations. The paper by Wandel and Klimenko compared the MMC to find that it produces favourable results (Wandel & Klimenko 2005). Therefore MMC can be deemed a useful and appropriate for the modelling of turbulent combustion.

A generalised MMC approach was developed by Cleary and Klimenko (2009) and effectively incorporates the mixture fraction based models, the pdf methods and DNS techniques into a single methodology. Although this approach is not designed for a partially stirred reactor it may be possible to take some aspects and apply them.

Vogiatzaki (2009) has successfully compared the MMC model with real life experimental turbulent reacting jets. It was concluded that the predictions for reactive species and temperature made by the model were in good agreement with the experimental data that had been gathered as well as agreeing with other models such as conditional moment closure. MMC was proven to provide a consistent and attractive alternate approach for modelling of turbulent reactive flows.

The model that is being used for this project was applied to a partially stirred reactor by Wandel (2005). Wandel's thesis develops the MMC model for applications in turbulent combustion. Overall the developments were deemed successful, however for a partially stirred reactor the MMC was decided as not appropriate as a loss of locality was caused. It was stated that this problem requires somewhat artificial corrections to the MMC formulations in an effort to obtain reasonable results.

The MMC model has also been applied to a partially stirred reactor by Sundaram (2013). In the paper the MMC model was used to predict extinction modes for turbulent premixed combustion. It was concluded that the MMC-PaSR model used is capable of simulating for premixed and non-premixed combustion however it requires the inclusion of more complex kinetics to predict temperature and species emissions.

2.4 MMC APPLIED TO PARTIALLY STIRRED REACTOR

This project analyses the simplified case of MMC applied to a partially stirred reactor. This case is favourable as it is a boundary value problem rather than an initial value problem so a stable convergence to the steady state solution is all that is required. MMC applied to a PaSR is a homogeneous case with an adiabatic combustion chamber at constant pressure. There are three key stages to the model, these are inflow/ outflow, mixing fractional step and reaction fractional step.

2.4.1 INFLOW AND OUTFLOW

The first stage models the fluid particles that are added and removed from the system. The particles are chosen randomly to be removed and new particles enter as either complete fuel or oxidiser. The number of particles replaced is defined as;

$$N_{replaced} = N * \frac{\Delta t}{\tau_{res}} \qquad (2.3)$$

Where N is the number of particles in the system, Δt is the time step and τ_{res} is the mean residence time (defined as, mass of fluid inside the reactor / mass inflow rate).

Of the replaced particles the amount that are fuel can be calculated as;

$$N_{r,fuel} = N_{replaced} Z_{in} \qquad (2.4)$$

The number of fuel particles is the total amount of replaced particles multiplied by the input mixture fraction. The remainder of the input particles will therefore be oxidiser. If $N_{replaced}$ or $N_{r,fuel}$ are not whole numbers then the value taken at any time step then will be the whole number above or below the actual value so that the mean number selected is satisfies the actual value.

When the new particles are added their life is reset to zero which results in an age distribution defined by the exponential equation;

$$f_{age}(s) = \frac{1}{\tau_{res}} \exp\left(-\frac{s}{\tau_{res}}\right) \qquad (2.5)$$

Where s is the age

The new particles enter with a set temperature, mixture fraction and boundary condition. The particles enter cold at a temperature of 300 Kelvin as either complete fuel or oxidiser ($Z = 1$ or 0). The boundary conditions dictate the reference space into which the new particles are added. The reference space that the particles are introduced into will effect how they mix with each other and the particles within the reactor.

2.4.2 MIXING FRACTIONAL STEP

The mixing step is where the MMC is applied to model the molecular mixing. The movement of the particle in the reference space is defined as;

$$d\xi = -Adt + \sqrt{2B}dt * R \qquad (2.6)$$

A = drift of the particle towards the mean (A=Bξ)

B = Diffusion, or normal molecular motion

R = Random normal variable

The diffusion coefficient 'B' should be selected so that its maximal value causes the terms of the MMC to dominate the influx/outflux term without making it insignificant. It can be found using;

$$B = \langle N \rangle / \langle \left(\frac{\partial Z}{\partial \xi} \right)^2 \rangle \qquad (2.7)$$

$\langle N \rangle$ = mean scalar dissipation rate

For homogeneous flow when the mixture fraction is plotted against the reference space the result is expected to have the form of the normal distribution. This is shown in Figure 1. The effects of the drift and diffusion both cause the particle to move along the reference space. Figure 2-1 demonstrates the expected distribution of particles throughout the reference space. The drift term will cause any particles to move towards the mean or as shown in figure 2-1, the solid line. The diffusion however is randomised as it resembles the normal molecular motion. This could cause the particle to move either direction in the reference space.

Another step in the mixing process sees particle pairs being selected depending on the location on the reference space. If particles are close to

another or deemed local they have the possibility of being paired together. The new values for each particle is then given as the arithmetic mean of the original values. This process is similar to the Modified Curl (MC) mixing method however the MC method can pair particles from anywhere within the reference space, whereas MMC can only pair with local particles.
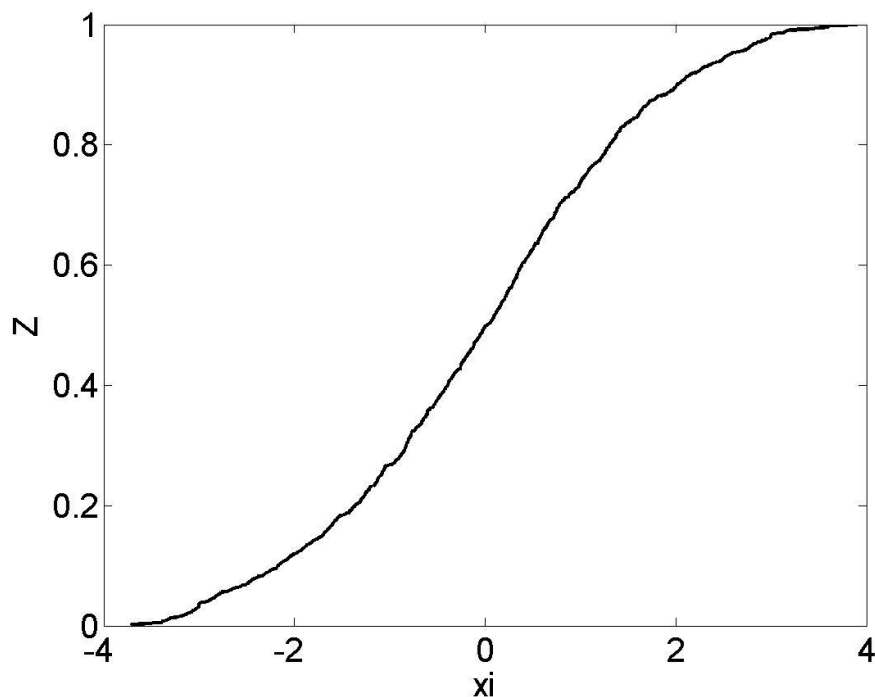
FIGURE 2-1 EXAMPLE PLOT, MIXTURE FRACTION VS REFERENCE VARIABLE

2.4.3 REACTION FRACTIONAL STEP

The final stage is the chemical reaction step. The chemical reaction is the process in which one set of chemical substances (the reactants) evolves into another (the products). These reactions can happen passively or can be catalysed by outside factors such as turbulence or heating. The changes occur to each particle according to the reaction equation over a time step of Δt. Each element has its own reaction equations for how it will interact with other

elements. The reaction mechanisms of a hydrogen and air system are shown in Table 1.

TABLE 1- H2/AIR REACTION MECHANISMS (MAAS & WARNATZ 1988)

		A	β	Ea
1.	$O_2 + H \leftrightarrow OH + O$	2.00×10^{14}	0.0	70.3
2.	$H_2 + O \leftrightarrow OH + H$	5.06×10^{4}	2.7	26.3
3.	$H_2 + OH \leftrightarrow H_2O + H$	1.00×10^{8}	1.6	13.8
4.	$OH + OH \leftrightarrow H_2O + O$	1.50×10^{9}	1.1	0.4
5.	$H + H + M \leftrightarrow H_2 + M$	1.80×10^{18}	-1.0	0.0
6.	$H + OH + M \leftrightarrow H_2O + M$	2.20×10^{22}	-2.0	0.0
7.	$O + O + M \leftrightarrow O_2 + M$	2.90×10^{17}	-1.0	0.0
8.	$H + O_2 + M \leftrightarrow HO_2 + M$	2.30×10^{18}	-0.8	0.0
9.	$HO_2 + H \leftrightarrow OH + OH$	1.50×10^{14}	0.0	4.2
10.	$HO_2 + H \leftrightarrow H_2 + O_2$	2.50×10^{13}	0.0	2.9
11.	$HO_2 + H \leftrightarrow H_2O + O$	3.00×10^{13}	0.0	7.2
12.	$HO_2 + O \leftrightarrow OH + O_2$	1.80×10^{13}	0.0	-1.7
13.	$HO_2 + OH \leftrightarrow H_2O + O_2$	6.00×10^{13}	0.0	0.0
14.	$HO_2 + HO_2 \rightarrow H_2O_2 + O_2$	2.50×10^{11}	0.0	-5.2
15.	$OH + OH + M \leftrightarrow H_2O_2 + M$	3.25×10^{22}	-2.0	0.0
16.	$H_2O_2 + H \leftrightarrow H_2 + HO_2$	1.70×10^{12}	0.0	15.7
17.	$H_2O_2 + H \leftrightarrow H_2O + OH$	1.00×10^{13}	0.0	15.0
18.	$H_2O_2 + O \leftrightarrow OH + HO_2$	2.80×10^{13}	0.0	26.8
19.	$H_2O_2 + OH \leftrightarrow H_2O + HO_2$	5.40×10^{12}	0.0	4.2

A units, mol cm s K; Ea units, kJ/mol; $k^+ = AT^{\beta} \exp(-E_a/RT)$, mol cm s K

2.5 LITERATURE REVIEW FINDINGS

After completing the literature review it has been found that there is not much existing literature on the specific topic of this project. There is lots of previous work in the combustion field involving various types of models, however for MMC specifically it is limited. This is most likely because the MMC method is relatively new and has only been used since around 2004. Other methods such as pdf modelling has been used for much longer and therefore it is expected that a wider range of literature will be available. It has also been noted that a majority of the previous work has been performed by the same people. A lot of the pdf mixing models are covered in Pope's works whereas the MMC methods have been mostly developed by Klimenko and Wandel. Because the literature is confined to the same sources it is probable that all the information is relevant and accurate.

There is sufficient literature to demonstrate the development of the MMC mixing method and the verification of the accuracy of its results. This is important as it ensures that MMC is capable of providing appropriate information and that it should be capable of achieving the aims of this project.

For the case of a partially stirred reactor there has been some previous work completed involving different mixing methods. Although many of these other methods do not directly apply to the model used in this project they are still useful resources as a comparison of results. For example in this case the paper by Ren and Pope (2004) is being used as a direct comparison of results. For a partially stirred reactor modelled using the MMC method the literature is very limited. Sundaram (2013) applied the MMC model to a PaSR however it was for premixed combustion and the analysis was focused on the extinction modes not on the particular behaviour. Another instance of MMC applied to PaSR is Wandel's thesis (2005). The model used in Wandel's thesis is the model that will be further developed throughout this project and therefore all of the previous findings and information is completely relevant and it is the most important literature source for this project.

3 METHODOLOGIES

The key methodologies for this project involve making the necessary changes to the coding of the multiple mapping conditioning model. The model is developed in MATLAB with the use of toolboxes such as Cantera. MATLAB is good for this type of modelling as it possess a high computational power and easy to use interface while the toolboxes provide additional features that can be applied for certain situations. A list of inputs are used to set the conditions for the model and these conditions need to be the same as those used in the paper by Ren and Pope to ensure the results are comparable.

3.1 INPUTS OF THE MODEL

To ensure that the results of the simulations are directly comparable with the model results found by Ren and Pope it is important that all the conditions are the same. These conditions are defined as the inputs for the model.

The combustion system uses Hydrogen and air and is a function of two time scales; the residence time scale and the mixing time scale. The input conditions state that the fuel and oxidiser are input cold and without any premixing. The fuel input has a volume ratio of one part nitrogen to one part hydrogen at 300 Kelvin, whereas the oxidiser is 79 parts oxygen to 21 parts nitrogen in order to represent the characteristic composition of atmospheric air. The reactor is at constant atmospheric pressure with the mass flow rate in equal to the mass flow rate out (i.e. $\dot{m}_{in} = \dot{m}_{out} = \dot{m}_{fuel} + \dot{m}_{ox}$). Due to the mass flow rate in being equal to the flow rate out the mass inside the reactor will be constant. The residence time scale can then be defined as;

$$\tau_{res} = m/\dot{m} \tag{3.1}$$

The residence time scale is the average time that any particle takes to complete its residence within the reactor. The inflow mixture fraction can be found as;

$$Z_{in} = \dot{m}_{fuel}/(\dot{m}_{ox} + \dot{m}_{fuel}) \tag{3.2}$$

From the molecular weights of the present elements and the composition of each particle the mixture fractions can be found. For the initial conditions all particles are at chemical equilibrium and sixty percent of all the particles are to be set to the stoichiometric mixture fraction.

For the figures developed by Ren and Pope to be directly comparable the resident time scale and mixing time scale need to be set to the values designated in the paper. For the figures given the resident time scale is, $\tau_{res} =$

$2e - 3$ and the relation between resident and mixing time scale is, $\tau_{mix}/\tau_{res} = 0.35$. These time scales are defined in the input variables for the function file. The string of input variables include:

klmfile-   Is the string or name of the chemical kinetics file

loadstr-   String or number to specify which initialisation file to use

t_f-   The total length of the simulation

tres-   The residence timescale

tmix_tres-   The ratio of mixing to residence timescale

Phi-   The equivalence ratio

mdot-   The total mass flow rate through the reactor chamber

alpha_v-   The variance of the mixing parameter generator used for
OLCM

np-   The number of particles

For this model the 'klmfile' and 'loadstr' are handled differently using Cantera for the chemical kinetics and the initialisation file being loaded independently. The number of particles is also defined in the initialisation file and although Ren and Pope use 1000 particles in their simulation changes to this will only change the amount of data gathered and therefore the accuracy without much effect to the actual results. For the simulations in this project 1000 particles were used to ensure accuracy. As stated the residence timescale was set to 2e-3 seconds and the mixing time scale is $0.35\tau_{res}$. The time step for the simulation is defined by Ren and Pope (2004) as a function of the smallest timescale,

$$\Delta t = 0.1 \times \min(\tau_{res}, \tau_{mix}) \qquad (3.3)$$

For some simulations the time step was decreased even further to ensure a high level of accuracy and to analyse the behaviour throughout the time. The

simulation runs for the residence time and therefore the number of time steps will be equal to $\Delta t / \tau_{res}$.

3.2 CHEMICAL REACTIONS

For this project Cantera is used for the chemical reactions. Cantera is a suite of software tools for problems involving chemical kinetics. It is a C++ based code with an interface in MATLAB. Useful features include the ability to assign conditions to a gas and then record details such as enthalpy or temperature and evolve the gas according to the reaction equation. The Cantera package does not include the reaction mechanism for combustion of hydrogen and air therefore a new 'cti' file had to be created to include the relevant information. The new file was adapted from the existing Cantera mechanisms and can be seen in Appendix C.

Cantera was used to solve each particle for chemical equilibrium in the initialisation. This required creating an ideal gas mix for each particle then assigning the mass fractions of each species to this gas. The equilibrate function was used to find the chemical equilibrium for that particle and then details such as temperature, mass fractions and density were recorded. Cantera was also used to run the chemical reaction stage of the model. This is done in a similar manner to solving for equilibrium in that a gas is created to resemble each particle. The gas was created using the updated cti file and was assigned values for pressure, mass fractions and enthalpy. A reactor was then created and set to remain at a constant pressure. The reactor network was formed and the created gas for each particle is inserted. The gas was advanced according to the reaction equations by the time of Δt and then the new values for mass fractions and temperature were recorded. This process was repeated each time step for each individual particle.

3.3 BOUNDARY CONDITIONS

The project objectives require changes to be made to the boundary conditions of the MMC model. When the model was first applied to a PaSR it was deemed not appropriate as there was a loss of locality. It is expected that this issue can be resolved by making some alterations to the boundary conditions. The boundary conditions of the model dictate how the new particle enter the system. Previously the boundary conditions were set that new particles would enter at all points throughout the reference space. This was done to try and maintain the probability distribution of the reference variable. Each particle was assigned a random value in the reference space that satisfied the probability density. It was theorised that by changing the boundary conditions the loss of locality that was experienced could be resolved. Therefore the boundary conditions were altered so that the new particles enter to the reference space at xi = 3 and -3 depending on mixture fraction. This means that fuel particles would be input into the single point in reference space where the mixture fraction is approximately one and oxidiser particles will enter where the mixture fraction is close to zero. The particles will then mix as defined by eq 2.6 and pair with other local particles. This will cause the particles to move towards the middle of the reference space where the fuel can mix with oxidiser.

3.4 TESTING AND VALIDATION

Once the initial simulations were completed further testing was performed to validate the model. Simulations were performed with changes to the residence time scale and mixing time scale to compare the behaviour with the expected result and test the limitations of the model. The residence time scale is the time that takes for one average residence to be completed. Therefore increasing this value will lead to the particles remaining with the reactor for on average a longer period of time. Also because new particles enter when

particles are ejected from the reactor an increased τ_{res} will lead to new particles being added less frequently. Decreasing the residence time scale will have the adverse effect with a shorter time spent within the reactor and therefore new particles added more frequently. The mixing time scale defines how long it takes for a certain level of mixing to be achieved. Increasing τ_{mix} will lead to a slower mixing process and decreasing it will cause faster mixing.

4 RESULTS

There are two key aspects of the results. The first includes the results that have been obtained to validate the model by directly comparing with the available literature. For the second aspect results have been obtained for a range of conditions for the residence time scale and the mixing time scale in order to further test the model and investigate the behaviour of the combustion system. The results for this part are to be compared with the expected results and although no direct comparison can be made it can be determined if the model responds to the changes of the time scales in the expected manner. For more plots developed from the simulation for the diffusion and temperature of the particles see appendix B.

4.1 COMPARISON OF RESULTS

The simulation was run multiple times using different random seeds. This was done to test the model and ensure that no errors were encountered. Five of the simulations are recorded in Appendix B and simulation B-1 is analysed here.

For the direct comparison of results with the simulations performed by Ren and Pope the initial condition were set to:

τ_{res} = 2e-3

τ_{mix} = 0.35 τ_{res}

Number of Particles = 1000

Number of Time Steps ≈100

4.1.1 ANALYSIS OF TEMPERATURE

Figure 4-1 shows the plot as developed by Ren and Pope using the Euclidean Minimum Spanning Tree model. The solid line shows the chemical equilibrium and the particles are shown below the curve. At the chemical equilibrium the particles composition will no longer change with time as it is completely burnt. All the particles below the curve are either in the process of burning or have failed to burn completely.

Figure 4-2 shows the plot of Temperature against mixture fraction for the simulation that was run. The plot shows the particles at the first and the last time steps of the simulation. At the first time step all the particles are at chemical equilibrium as per the initial conditions and therefore a distinct line is made. The particles at the final time step show how much extinction has occurred over the length of the simulation which is the average residence time.
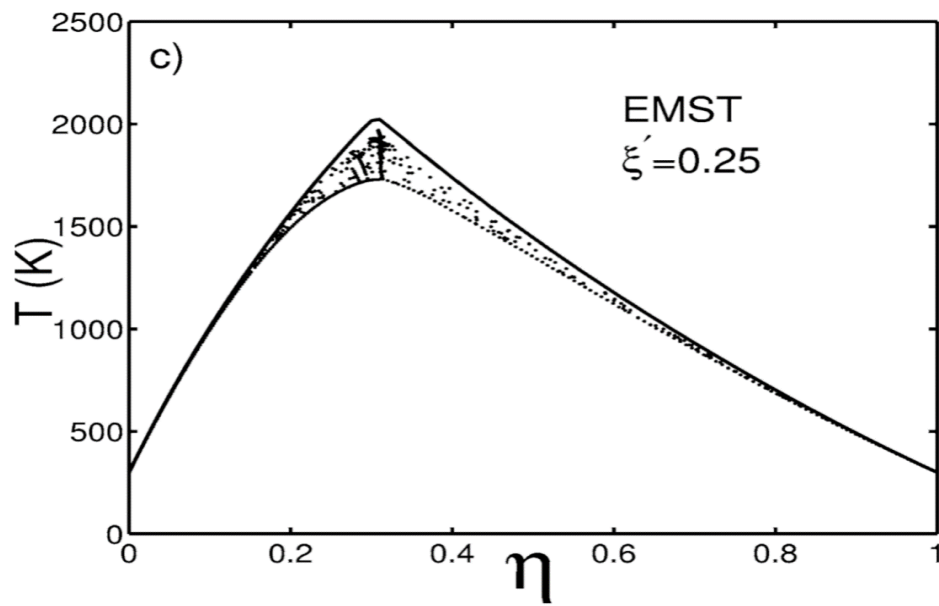
FIGURE 4-1 - TEMP VS MIXTURE FRACTION, COMPARISON PLOT GENERATED BY REN AND POPE (2004)
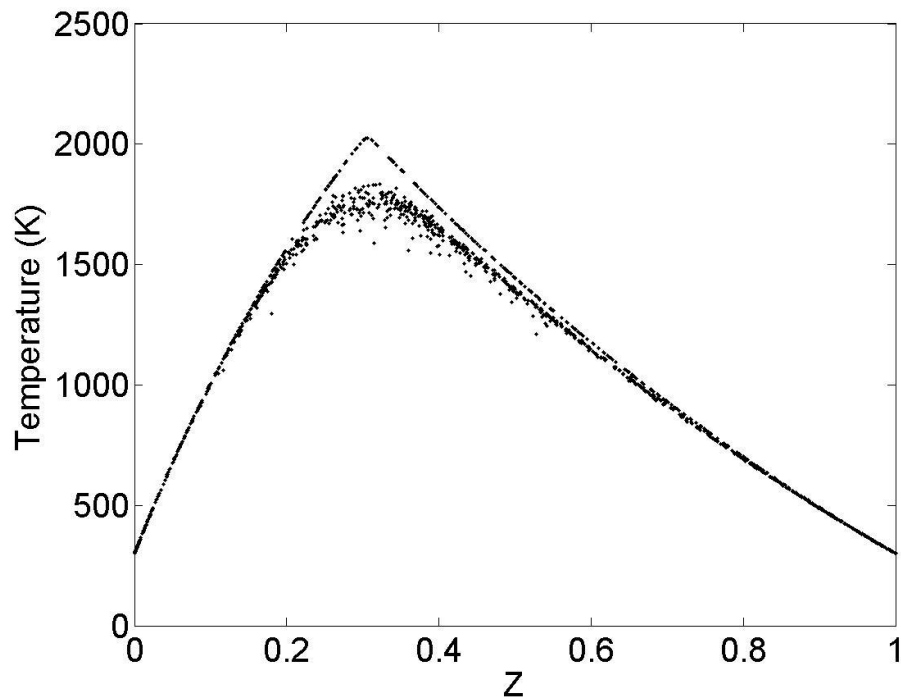
FIGURE 4-2 - TEMP VS MIXTURE FRACTION, ORIGINAL CONDITIONS; T_{RES} = 2E-3, T_{MIX} = 0.35 T_{RES}

4.1.2 ANALYSIS OF MIXING AND DIFFUSION

To analyse the mixing of the model and the dispersion of the particles throughout the reference space the mixture fraction is plotted against the reference variable. General diffusion will have the shape of an error function where the reference space at either end has a mixture fraction of zero or one with the highest rate of change around where xi is equal to zero.

Figure 4-3 shows the individual particles with their mixture fraction and the location in the reference space. This plot was generated at the final time step and therefore demonstrates the final level of diffusion that the simulation achieves.
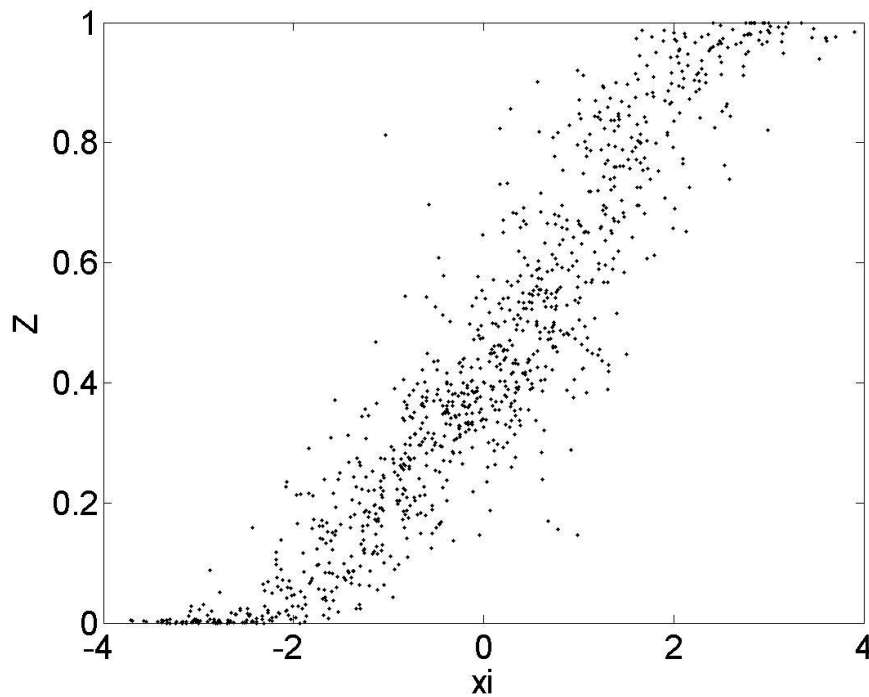
FIGURE 4-3 - DISPERSION OF PARTICLES IN REFERENCE SPACE, ORIGINAL CONDITIONS, $T_{RES} = 2E-3$, $T_{MIX} = 0.35$ T_{RES}

Figure 4-4 shows the reference variable sorted in ascending order and then plotted against values from zero to one for the number of particles to represent the mixture fraction. This creates a curve that shows the nature of the diffusion throughout the reference space and can be used to analyse the mixing.
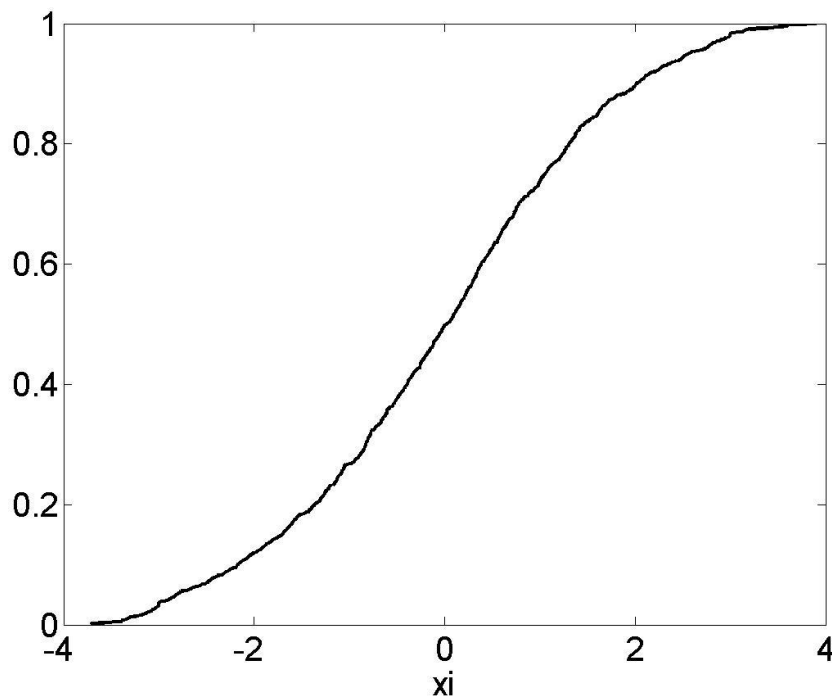
FIGURE 4-4 – REFERENCE VARIABLE PROFILE, ORIGINAL CONDITIONS, T_{RES} = 2E-3, T_{MIX} = 0.35 T_{RES}

4.1.3 DISCUSSION

The initial results for the simulation with the same conditions as Ren and Pope's EMST model demonstrate positive signs for the MMC model. The general shape of the curve in Figure 4-2 is very similar to Figure 4-1 and therefore suggests that the model is viable for the case of a partially stirred

reactor. Of particular notice is the amount of particles that have fallen below the chemical equilibrium curve and the location along the curve that they occur. The key differences that can be noticed between the MMC model and the EMST model are that the particles in the MMC model fall a bit further below the equilibrium curve at the peak. However the majority of particles in the EMST model fall in the same range as the MMC model from around 1600 Kelvin to 1800 Kelvin at the peak. Another difference that can be noticed is that the MMC model shows a few particles that are further below the rest. This is likely because those particles are still in the process of burning and will increase in temperature as they burn more completely. Apart from these differences the MMC model produces results that are very similar to the EMST model suggesting that it is a viable model for a partially stirred reactor. For a more reliable comparison, direct numerical simulations could be used for the same conditions and compared with the MMC results.

The diffusion curves demonstrates positive results for the mixing of the model. The distribution shows that the mixing is causing the diffusion throughout the reference space and the new particles are mixing with the particles within the reactor. The diffusion is steady with a fairly even amount of particles spread across the reference space without any excessive concentration of particles at the input variables.

This method of validation is only comparative with the accuracy depending on the comparison to the EMST model. Although this comparison is not entirely identical it does demonstrate that the MMC model provides results that are very similar. As the EMST model is not completely accurate it cannot be declared that the MMC model is more or less correct. For a more accurate comparison direct numerical simulations could be used with the same conditions as the MMC model.

It was found that occasionally the simulation encounters an error with the chemical reactions where the particle cannot be advanced by the reaction equation. This is generally solved by changing the size of the time step.

Decreasing the time step made it so that the reaction solver did not have to advance the particle as far and was able to step through the reaction mechanics. This issue was more prevalent in simulations with altered time scales and therefore it could be caused by the different conditions.

4.2 INCREASED RESIDENCE TIME SCALE

A number of simulations were run with an increased residence time scale. This was done to experiment with the conditions and see if the model will handle the changes in the expected manner. Also the limitations of the model can be found.

Three different residence time scales were used and all other conditions remained the same as the initial simulations so that comparisons can be made. Conditions for these simulations are:

τ_{res} = 7e-3, 2e-2 and 7e-2

τ_{mix} = 0.35τ_{res}

Number of Particles = 1000

Number of Time Steps ≈100

4.2.1 ANALYSIS OF TEMPERATURE

Figures 4-5 to 4-7 show the temperature plots for the increased residence time scales. Simulations were run with three different residence time scales at 7 milliseconds, 20 milliseconds and 70 milliseconds. These values are used to give a good demonstration of how the results change with the increasing timescale.
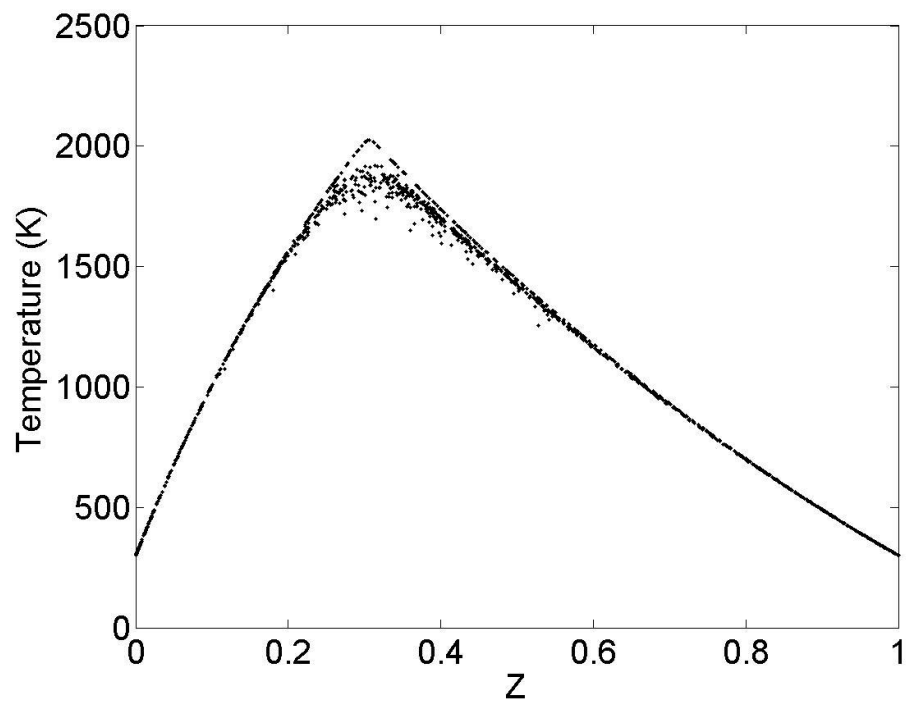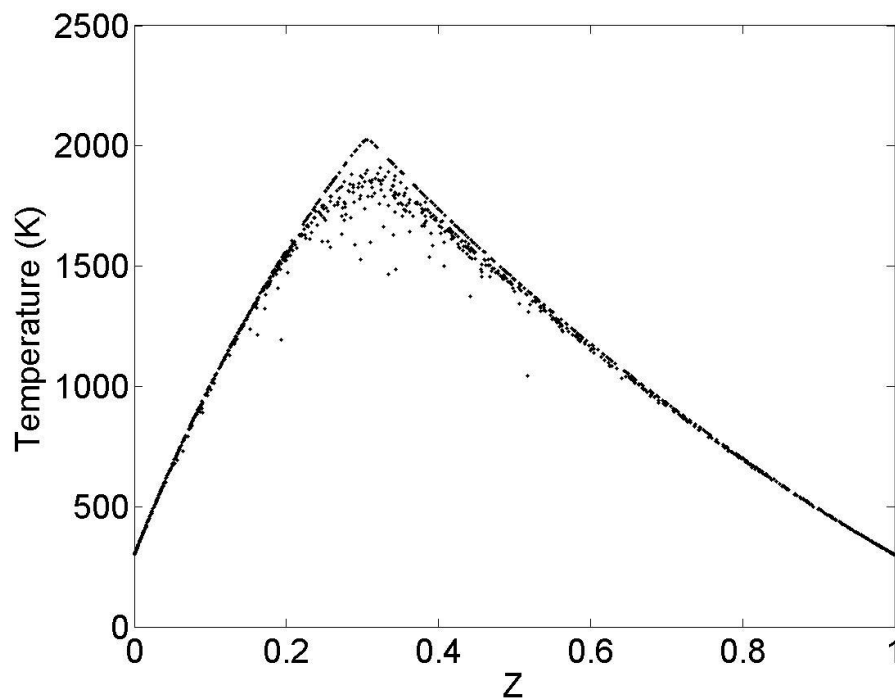
FIGURE 4-5 - TEMP VS MIXTURE FRACTION, INCREASED RES; T_{RES} = 7E-3,

T_{MIX} = 0.35 T_{RES}
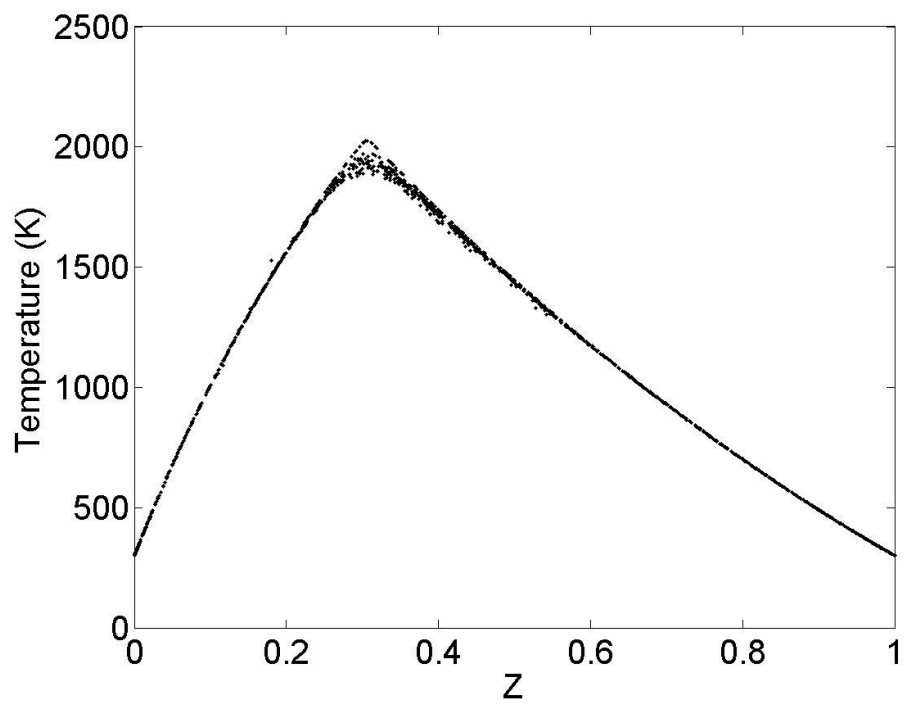
FIGURE 4-6 - TEMP VS MIXTURE FRACTION, INCREASED RES; T_{RES} = 2E-2,

T_{MIX} = 0.35 T_{RES}

4.2.2 ANALYSIS OF MIXING

Figure 4-8 shows the diffusion of particles for the highest residence time scale of 70 milliseconds. This plot is used to demonstrate that the diffusion of the particles will not change with the increasing time scale. This is because the mixing time scale is set as a fraction of the residence time scale and therefore the relationship remains the same.
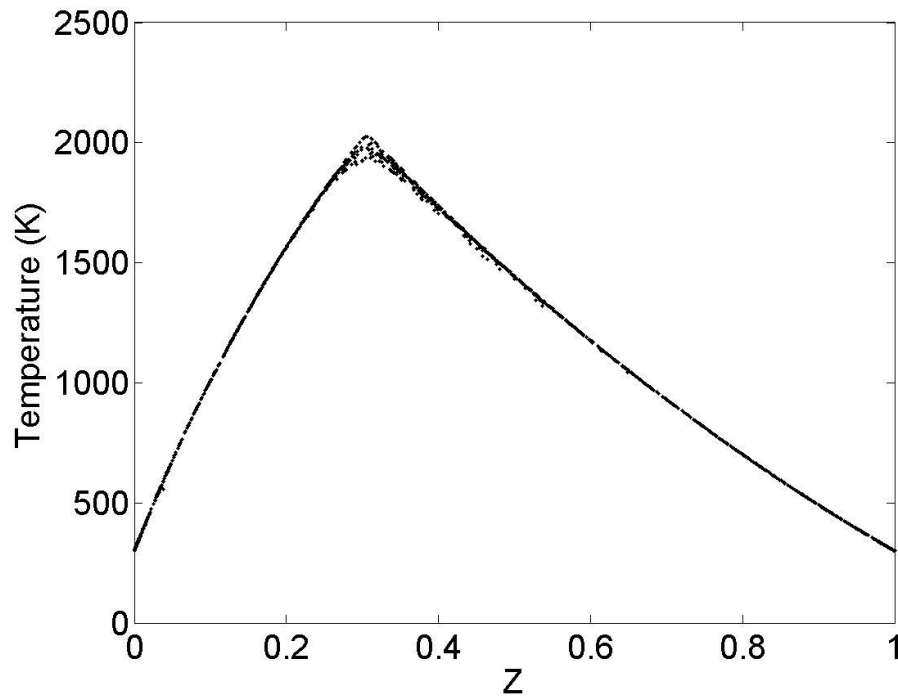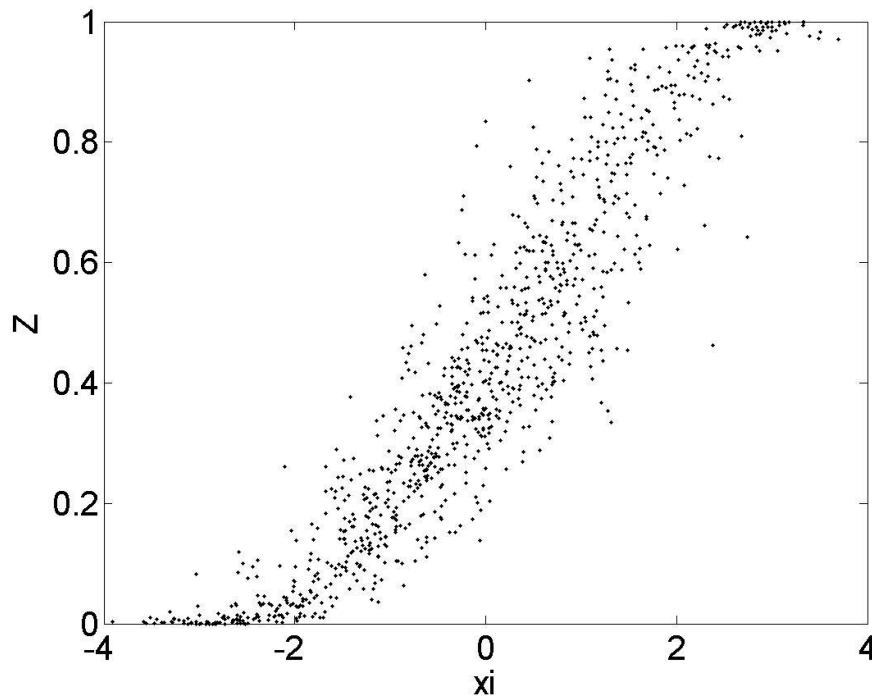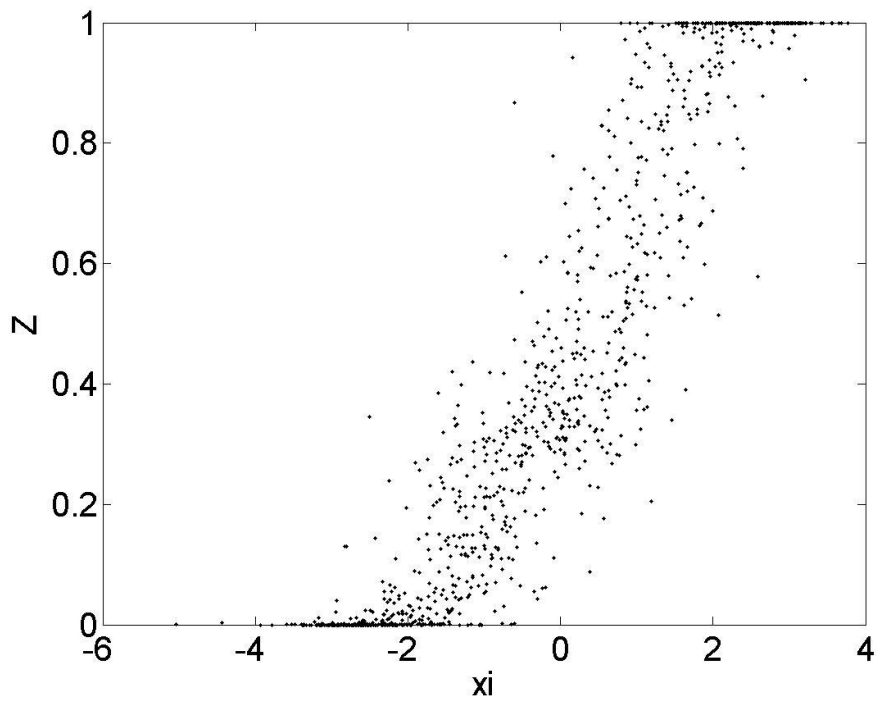
FIGURE 4-8 - DISPERSION OF PARTICLES IN REFERENCE SPACE, INCREASED RES, $T_{RES} = 7E-2$, $T_{MIX} = 0.35$ T_{RES}

4.2.3 DISCUSSION

From Figures 4-5 to 4-7 it can be seen that as the residence time scale increases the amount of local extinction and unburnt particles decreases. Increasing the residence time scale means that the particles take a longer time to complete an average residence and therefore spend a longer period of time within the reactor. This causes more complete combustion as the particles have more time to burn completely. Furthermore new particles are added less frequently and as the new particles are added cold they will decrease the temperature inside the reactor while mixing.

The diffusion curve will not change with the increased residence time scale. This is because the diffusion is mostly effected by the mixing process and the mixing time scale is not altered for these simulations. The mixing time scale

40

is set as a fraction of the residence time scale and therefore will automatically adjust to the changes in the residence time scale. Both the diffusion curve and the dispersion of particles closely resemble the original simulations and can be seen in Appendix B.

There are limitations to how large the residence time scale can be set. By gradually increasing the residence time scale it was found that at a time of approximately one second there is almost no extinction. Increasing it beyond this causes all particles to eventually reach the chemical equilibrium until a residence time scale of about two seconds where the chemical reaction solver encounters an error. The error is caused due to the particle not being able to evolve according to the reaction equations. These limitations could be due to the reactants completely burning faster than the new particles are entering the system and therefore all the reactants are used up and there is not enough fuel and oxidiser entering to maintain the combustion.

4.3 DECREASED RESIDENCE TIME SCALE

Three different decreased residence time scales were used to further analyse and investigate the behaviour of model. All other conditions remained the same as the initial simulations so that comparisons can be made. Conditions for these simulations are:

τ_{res} = 2e-4, 7e-5 and 2e-5

τ_{mix} = 0.35 τ_{res}

Number of Particles = 1000

Number of Time Steps ≈100

4.3.1 ANALYSIS OF TEMPERATURE

Figures 4-9 to 4-11 show the temperature plots for the decreased residence time scales. Simulations were run with three different residence time scales at 2e-4, 7e-5 and 2e-5
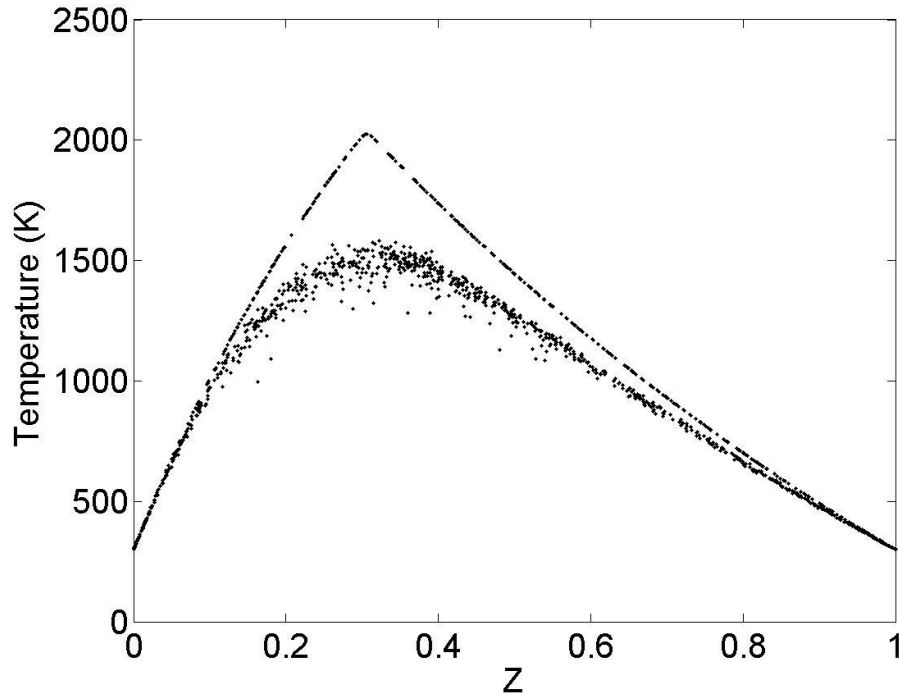
FIGURE 4-9 - TEMP VS MIXTURE FRACTION, DECREASED RES; $T_{RES} = 2E-4$, $T_{MIX} = 0.35$ T_{RES}
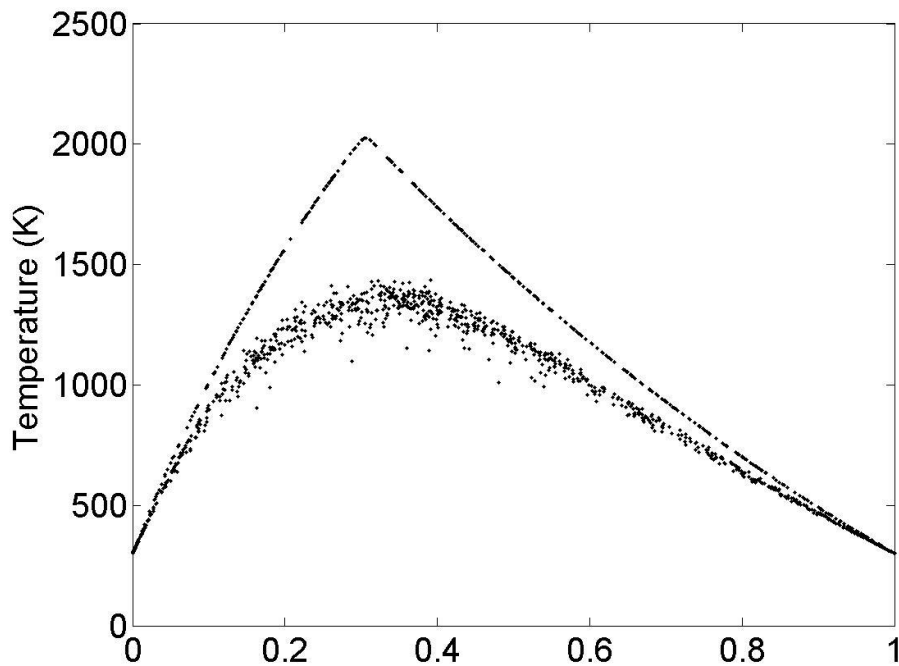
FIGURE 4-10 - TEMP VS MIXTURE FRACTION, DECREASED RES; $T_{RES} = 7E-5$, $T_{MIX} = 0.35$ T_{RES}
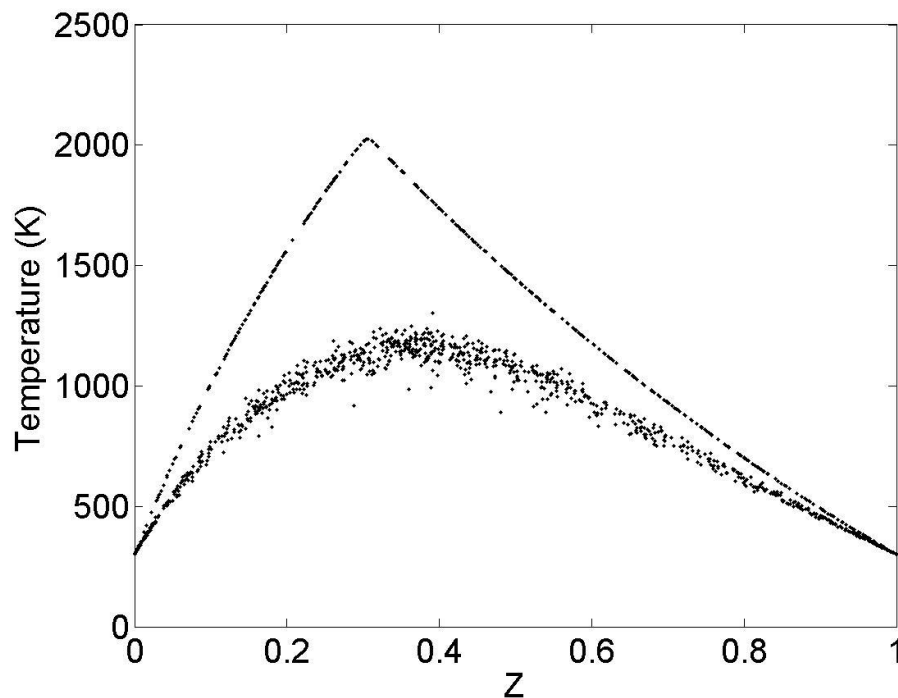
FIGURE 4-11 - TEMP VS MIXTURE FRACTION, DECREASED RES; $T_{RES} = 2E\text{-}5$, $T_{MIX} = 0.35$ T_{RES}

4.3.2 DISCUSSION

As the residence time scale decreases there is more local extinction of the particles and the temperature drops. The drop in temperature is likely due to the particles not having enough time within the reactor to combust completely. Also due to the residence being short there will be new particles being ejected more frequently. This could also cause a decrease in the overall temperature as the new particles enter cold at 300 Kelvin.

There will be no change to the diffusion curve because the mixing time scale is set to be a fraction of the residence time scale and will adjust to the changes that were made. Therefore the diffusion in not analysed however the plots can be seen in Appendix B.

By constantly decreasing the residence time scale it was found that any smaller than a value of τ_{res} = 2e-5 seconds does not greatly effect the temperature of the unburnt particles. The model is limited by memory requirements with the smallest successfully simulated time scale being 9e-6 seconds. Anything smaller than τ_{res} = 1e-7 seconds encounters an error with the memory required for processing. It may be possible to solve this error using a more powerful computer however the results will not change much beyond that point. For a real life combustion system it will reach a point where the particles do not have enough time sustain the chemical reactions. This will cause the global extinction and combustion will no longer be maintained.

4.4 INCREASED MIXING TIME SCALE

For these simulations the residence time scale was left the same as the original simulations at 2 milliseconds and the mixing time scale was increased. Therefore the mixing takes a longer amount of time to complete and the mixing process is more relaxed.

Three different mixing time scales were used and all other conditions remained the same as the initial simulations so that comparisons can be made. Conditions for these simulations are:

τ_{res} = 2e-3

τ_{mix} = 0.55, 0.75 and 0.95 τ_{res}

Number of Particles = 1000

Number of Time Steps ≈100

4.4.1 ANALYSIS OF TEMPERATURE

Figures 4-12 to 4-14 plot the temperature against the mixture fraction for the three increased mixing time scales and the original conditions. A steady change can be seen in the plots as the amount of particles under the chemical equilibrium decreases as the mixing time scale increases.

4.4.2 ANALYSIS OF MIXING

Figure 4-16 shows the reference variable profile for the simulations with higher mixing time scale. As the mixing time scale increases the curve becomes more linear. Figure 4-17 shows the particles diffusion in the reference space and demonstrates a similar behaviour to figure 4-16 as there are a higher amount of particles around the extremes of the mixture fraction.

FIGURE 4-12 - TEMP VS MIXTURE FRACTION, INCREASES MIX; $T_{RES} = 2E-3$, $T_{MIX} = 0.55$ T_{RES}
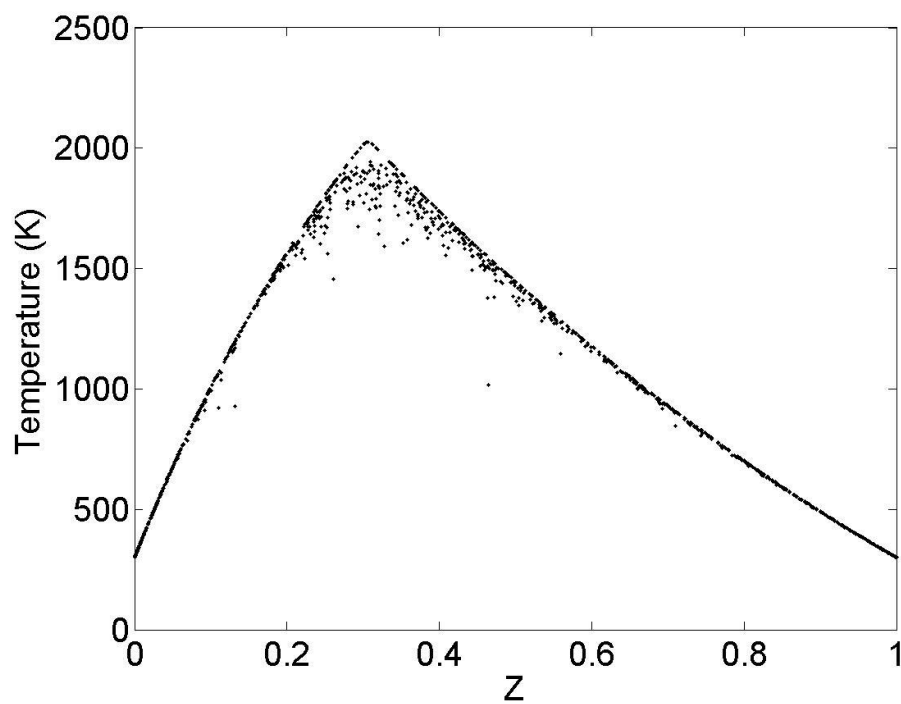
FIGURE 4-13 - TEMP VS MIXTURE FRACTION, INCREASED MIX; T_{RES} = 2E-3, T_{MIX} = 0.75 T_{RES}
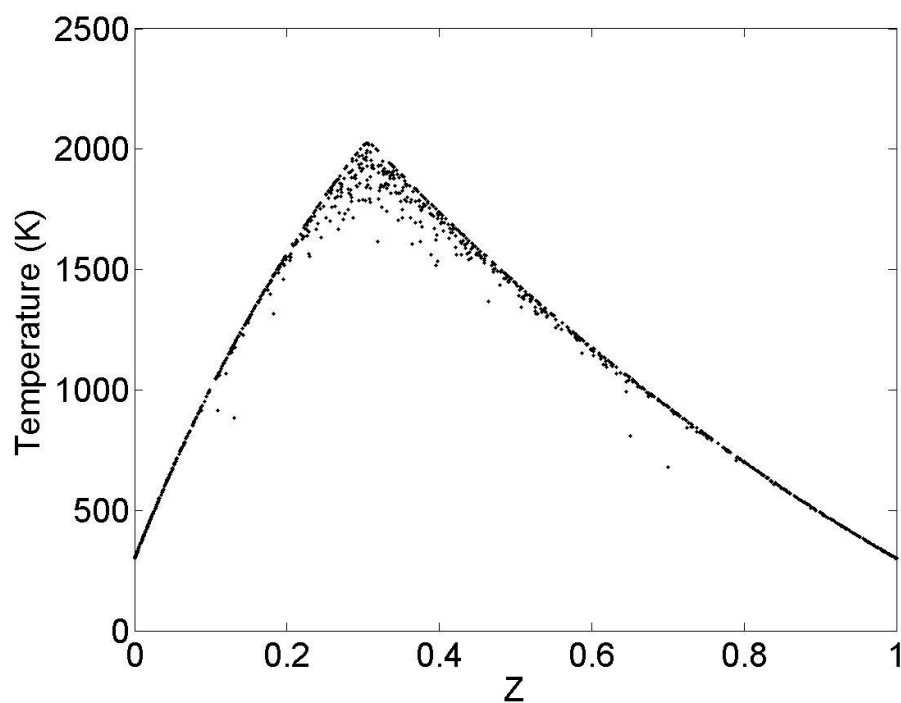
FIGURE 4-14 - TEMP VS MIXTURE FRACTION, INCREASED MIX; T_{RES} = 2E-3, T_{MIX} = 0.95 T_{RES}
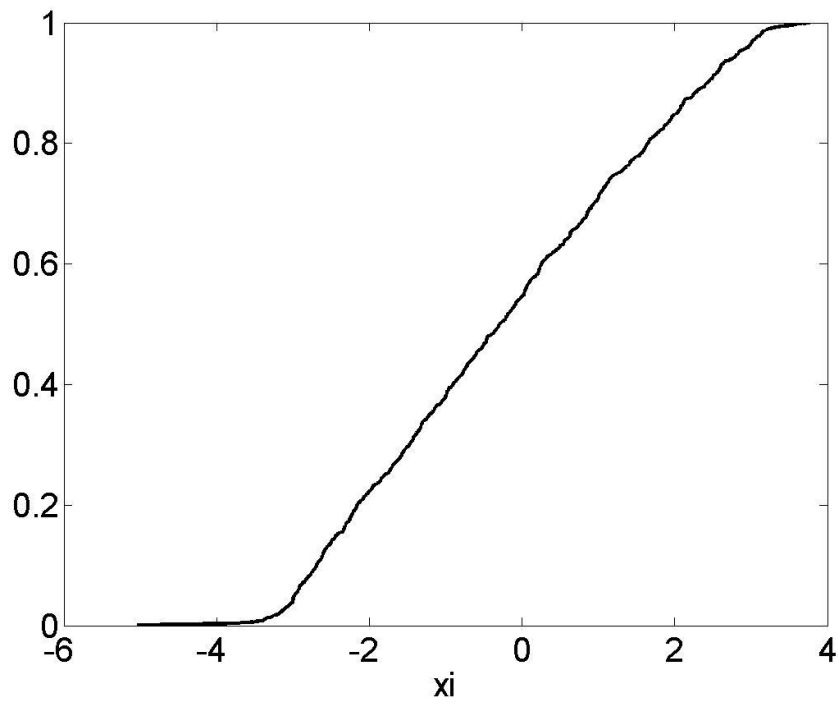
FIGURE 4-16 - REFERENCE VARIABLE PROFILE, INCREASED MIX, $T_{RES} = 2E$-3,

$T_{MIX} = 0.95 \ T_{RES}$

FIGURE 4-15 - DISPERSION OF PARTICLES IN REFERENCE SPACE, INCREASED MIX,

$T_{RES} = 2E$-3, $T_{MIX} = 0.95 \ T_{RES}$

4.4.3 Discussion

As the fraction of mixing time scale was increased the particles under the chemical equilibrium curve increase in temperature. However the mixing curve shows that the amount of particles around the stoichiometric mixture fraction is significantly less than the original simulations. Therefore the increased temperature of the particles could be due to the slow mixing allowing the particles to burn more completely without being effected by colder particles mixing in. The slower mixing also leads to the situation as seen in figure 4-14 where there are some particles further from the equilibrium curve. This is because they are not being combined with the hotter particles and therefore cannot react. These particles will remain at the same temperature until they do mix or are ejected.

The diffusion of the particles shows that there is a higher concentration of particles where the mixture fraction is either zero or one. This is due to the decreased mixing speed meaning that new particles that are added are not going to mix in with each other and the particles throughout the rector as quickly. Therefore more of the new particles will remain as either complete fuel or oxidiser for a longer period of time. The diffusion curve shows a similar behaviour as the higher concentrations of particles at the ends of the reference space cause the curve to become more linear. The curve being linear shows that the mixing is occurring slower and the dispersion of particles through the reference space is fairly even as opposed to the particles mixing towards $xi = 0$.

The mixing time is limited as global extinction will be reached when the mixing time is too long for a sufficient amount of mixing to occur. The MMC model is limited to a mixing time scale of $1*\tau_{res}$ if it is increased beyond this point the mixing does not have sufficient time to complete. Due to the initial conditions stating everything is at chemical equilibrium a large mixing time scale means the particles do not have time to mix with the new particles and

therefore extinction would occur as all the particles are either completely burnt or cold.

4.5 DECREASED MIXING TIME SCALE

The final set of simulations were run with a decreased mixing time scale. The mixing time scale was set to 0.25, 0.15 and 0.05 multiplied by the residence time scale. The changes will mean the mixing occurs much faster.

Conditions for these simulations are:

$\tau_{res} = 2e\text{-}3$

$\tau_{mix} = 0.25, 0.15 \text{ and } 0.05 \ \tau_{res}$

Number of Particles $= 1000$

Number of Time Steps $\approx 100\text{-}200$

4.5.1 ANALYSIS OF TEMPERATURE

Figures 4-17 to 4-19 plot the temperature against mixture fraction for the decreased mixing time scales. There is no great of difference in the amount of particles that fail to burn completely or their temperature however differences can be seen in the grouping of the unburnt particles and that the highest concentration of the particles under the curve has moved toward a higher mixture fraction.
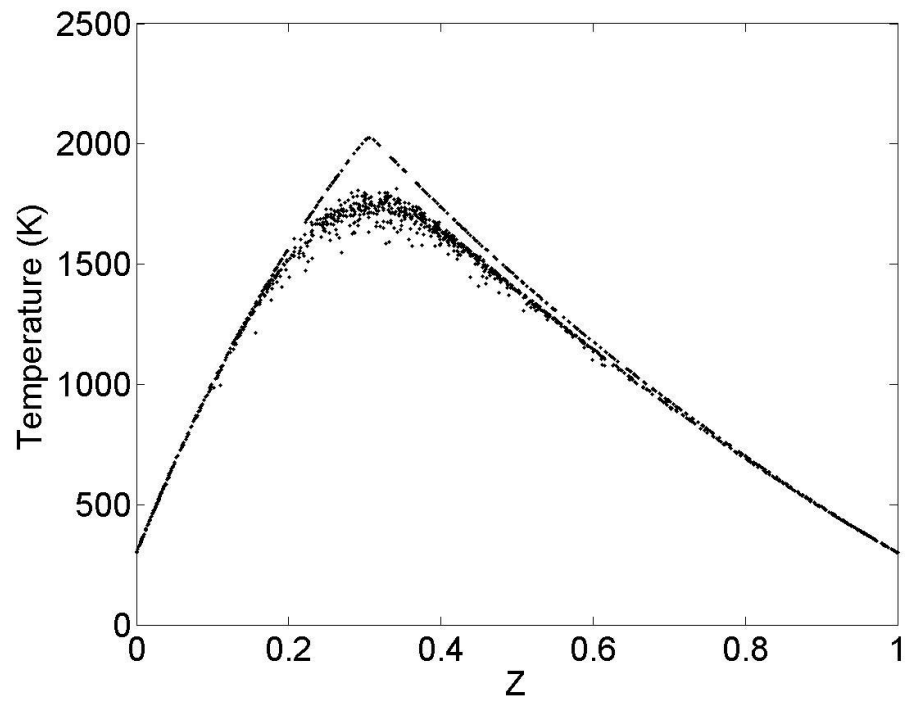
FIGURE 4-17 - TEMP VS MIXTURE FRACTION, DECREASED MIX; T_{RES} = 2E-3, T_{MIX} = 0.25 T_{RES}
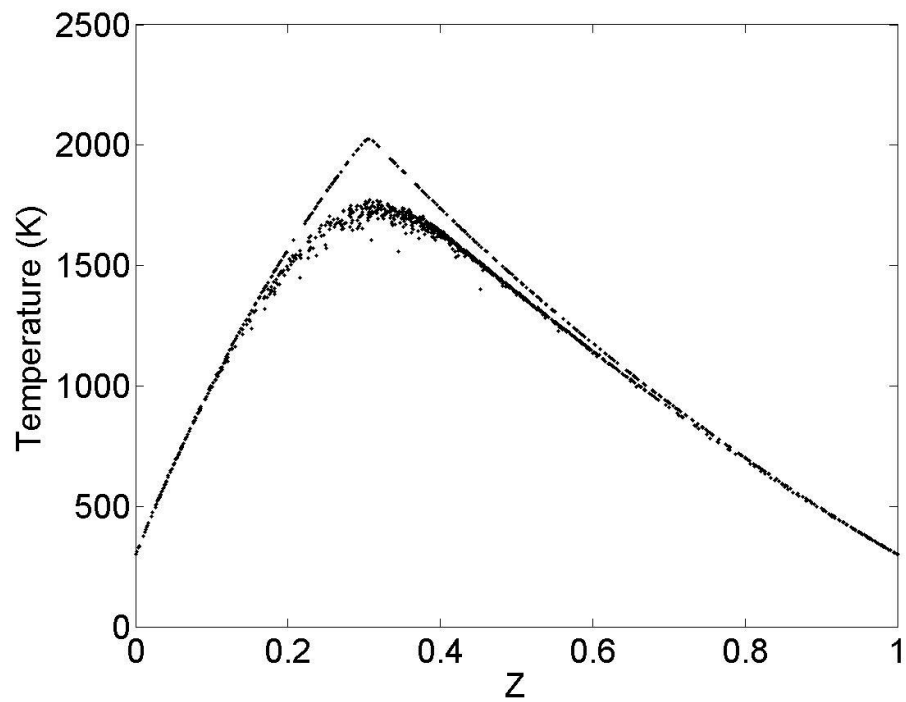
FIGURE 4-18 - TEMP VS MIXTURE FRACTION, DECREASED MIX; T_{RES} = 2E-3, T_{MIX} = 0.15 T_{RES}
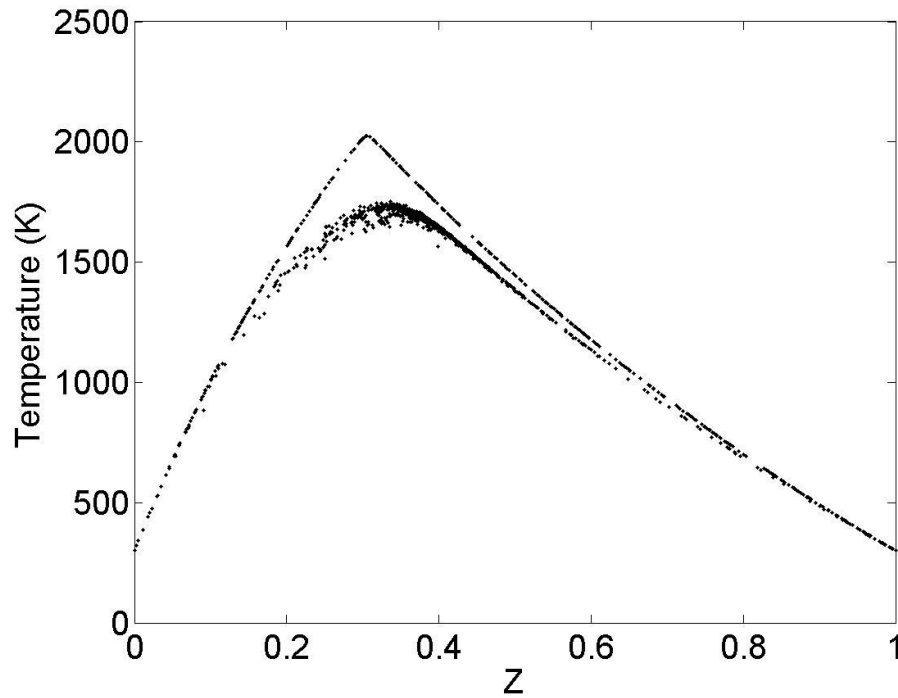
FIGURE 4-19 - TEMP VS MIXTURE FRACTION, DECREASED MIX; $T_{RES} = 2E\text{-}3$, $T_{MIX} = 0.05$ T_{RES}

4.5.2 ANALYSIS OF MIXING

Figure 4-21 demonstrates the diffusion of the particles for the simulations with a decreased mixing time scale. The original simulation is compared to the smallest mixing time scale to show the most extreme difference. Particles plotted against the reference variable are shown and demonstrate how to more intense mixing causes more particles to group in the middle of the reference space. Figure 4-20 demonstrates that due to the shorter time scale and more turbulent mixing the gradient in the middle of the curve increases. This is because there are more particles in the reference space around xi = 0.

51
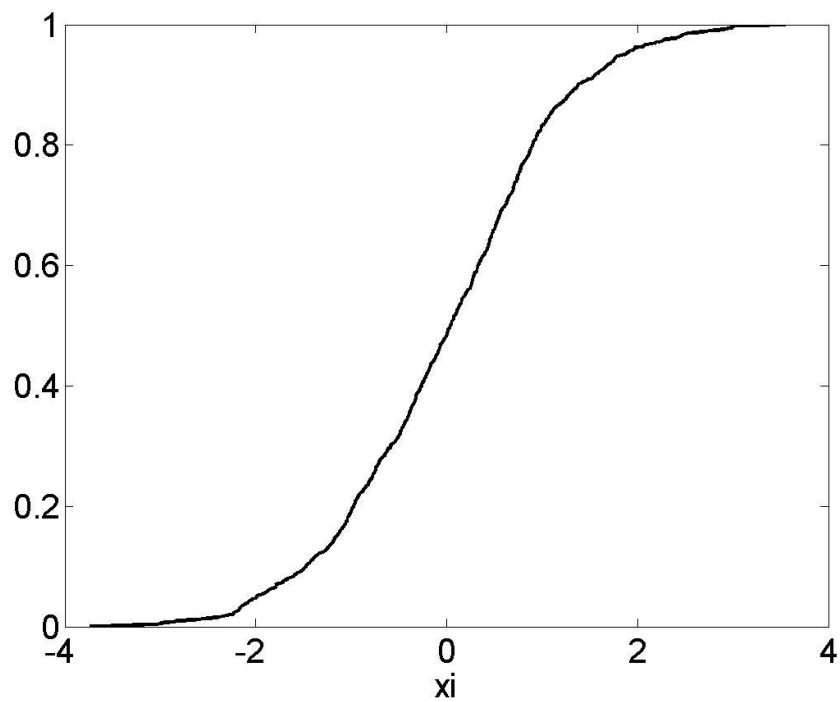
FIGURE 4-20 - REFERENCE VARIABLE PROFILE, DECREASED MIX, T_{RES} = 2E-3, T_{MIX} = 0.05 T_{RES}
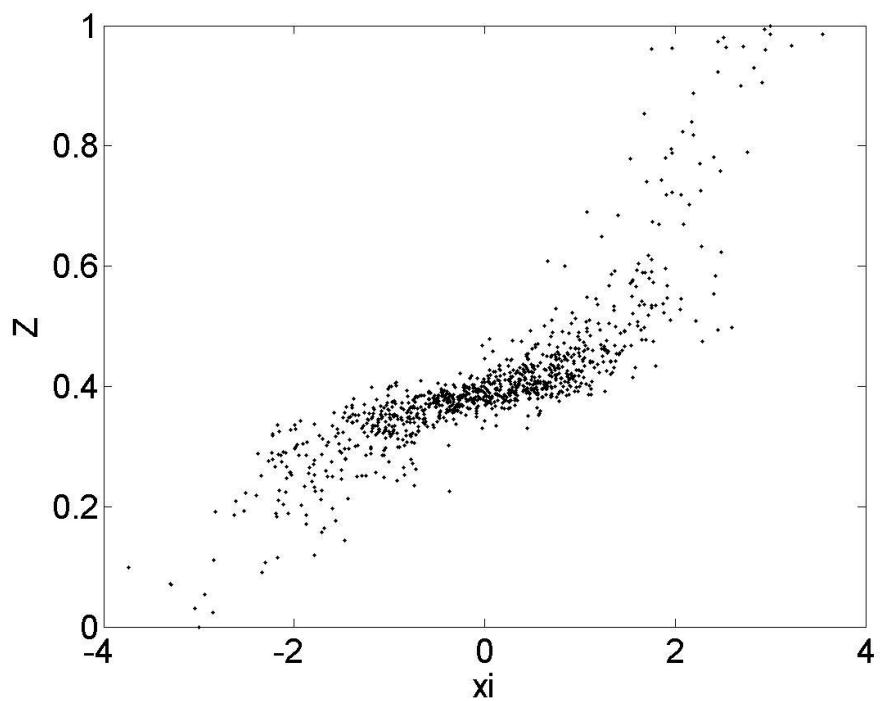
FIGURE 4-21 - DISPERSION OF PARTICLES IN REFERENCE SPACE, DECREASED MIX, T_{RES} = 2E-3, T_{MIX} = 0.05 T_{RES}

4.5.3 DISCUSSION

Figures 4-17 to 4-19 show that as the mixing time scale decreases there is not much change in the temperature of the particles under the chemical equilibrium. The most notable difference is that there is a greater number of particles and they are more concentrated. This is because the mixing process is faster causing the particles to mix rapidly and therefore end up with more similar compositions.

This behaviour is demonstrated with the diffusion of the particles. The particles can be seen to group together around the middle of the reference space with very few near the inlets of fuel and oxidiser. With the high mixing speed all the new particles that are added will very quickly mix together and move through the reference space resulting in very few particles at either end. The reference variable profile also shows that a lot of the particles are around xi = 0 in the reference space and therefore the gradient at this point is much higher.

Decreasing the mixing time scale is limited by approaching zero and computational power. As the time scale is decreased smaller time steps are required to accurate simulate. Due to the residence time scale staying the same smaller time steps means there will be more steps in the simulation and therefore more computational time is required.

5 CONCLUSIONS AND FUTURE WORK

5.1 CONCLUSION

Numerous simulations have been performed with various conditions in order to validate and test the MMC model applied to a partially stirred reactor. The EMST model from the paper by Ren and Pope was used for comparison as well as comparisons with the expected results.

Literature involving combustion modelling and in particular Multiple Mapping Conditioning was investigated to identify previous work and to study the model. It was found that there is not much literature available for the case of MMC applied to a partially stirred reactor with the majority of previous work performed by Wandel or Sundaram. Previous works from Wandel (2005) and Klimenko (2003) provided an understanding of the formulation of the MMC model and its development. Deterministic and stochastic formulations of MMC were analysed finding that the stochastic formulation is preferable when the dimensionality of reference space is large (i.e. ≥ 3).

The chemical reaction solver was updated to use the Cantera toolbox for MATLAB. Cantera provides a more simplistic approach than the previous methods and results in an easier to use model. The chemical reactions were altered to use the same mechanisms as Ren and Pope (2004) and ensure comparison was accurate.

In order to resolve the issues that had arisen in the previous work on the MMC applied to PaSR the boundary conditions of the model had to be altered. The boundary conditions were changed to introduce the new particles at given points in the reference space as opposed to the previous work that dispersed them throughout. It was changed so that the new particles enter at xi = -3 and 3 where the mixture fraction of diffusion curve is near zero and one.

Initial simulations were performed using the same conditions as Ren and Pope to make a direct comparison. The conditions for these simulations were a residence time scale of 2e-3, mixing time scale of $0.35\tau_{res}$ and 1000 particles. The temperature is plotted against mixture fraction to demonstrate the behaviour of the particles with the amount of local extinction being analysed. The plot shows that the particles fall under the chemical equilibrium to a minimum temperature of approximately 1600 Kelvin around the stoichiometric mixture fraction. The EMST model provides very similar results with the main difference being that the particles under the chemical

equilibrium reach a higher temperature of around 2000 Kelvin. While the results are not exactly the same as previous literature there is sufficient similarity to suggest the model is viable and appropriate to the real life expectations.

To further verify the model the random seed of the simulation was changed multiple times to ensure that the model still simulated successfully and provided similar results. For all simulations the results were very similar with no noticeable changes between each simulation. This also tested that the model is robust enough to manage the changes.

The next stage in validating the model involved simulating for a range of conditions and comparing with the expected behaviour. The values of residence time scale and mixing time scale were increased and decreased to experiment and observe the behaviour.

The res time scale was increased to 7e-3, 2e-2 and 7e-2 seconds. Increasing the residence time scale lead to the particles burning more completely. As the time scale is increased the amount of particles under the chemical equilibrium decreases until a point where almost all particles burn completely. This is due to the longer amount of time that the particles have within the reactor to mix together and evolve according to the chemical reactions. The mixing analysis showed no difference as the mixing time scale is the same fraction of the residence time scale.

Simulations were performed with a decreased residence time scale at 2e-4, 7e-5 and 2e-5 seconds. The decreased time scale caused a large increase in the amount of local extinction as the unburnt particles drop down to around 1100 Kelvin. This is as expected and the system will reach a point of global extinction when there is not enough time for the particles within the reactor to evolve according to the reaction equations. As with the increased residence time scale there is no difference in the diffusion of the particles as the mixing is relative to the residence.

The mixing time scale was increased to $0.55\tau_{res}$, $0.75\tau_{res}$ and $0.95\tau_{res}$. Changing the mixing time scale had some effect on the temperature and local extinction of the particles however was not as great as altering the residence time scale. By increasing the mixing time scale the mixing process takes a longer time and therefore the mixing is more relaxed. This leads to the particles burning more completely around the stoichiometric mixture fraction, however the main difference of the mixing time scale is shown in the diffusion plots. With a higher mixing time scale the mixing is slower and therefore the new particles added to the system take longer to mix with other particles. This behaviour is as expected and if the mixing time scale is too large global extinction would occur as there is not enough time for sufficient mixing to occur.

The final simulations that were run used decreased mixing time scales of $0.25\tau_{res}$, $0.15\tau_{res}$ and $0.05\tau_{res}$. As with the increased mixing time scale there was not a great difference in the temperature profile with the major difference shown in the diffusion of the particles. The diffusion of the particles shows that the high rate of mixing causes the particles to mix together very rapidly with the concentration being around the middle of the reference space.

In conclusion the simulations that were performed provided promising results for MMC applied to a PaSR. The results obtained from the simulations are similar to those of the previous literature and correspond with the expected behaviour.

5.2 FUTURE WORK

5.2.1 Future work for MMC applied to PaSR

For the further development of the MMC model applied to a partially stirred reactor more validation of the model could be performed. The model has been proven to produce realistic results and to behave in the expected manner. These tests have all been comparative with other models and the expected behaviour and therefore to test the accuracy of this model more accurate simulations such as direct numerical simulations could be applied for this specific case.

Other testing could also be performed by using completely different conditions such as other fuels. This would validate that the model is able to handle a range of conditions and is important so that it can be applied in various situations.

5.2.2 Future work for MMC

Future work for the multiple mapping conditioning model could include the application of the model to other real life cases. This project focused on the MMC model applied to a partially stirred reactor and MMC has been applied to a partially stirred plug flow reactor with some success by Wandel (2005). As the MMC model continues to developed and be proven accurate it could be applied to other situations to provide a more advanced modelling approach.

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APPENDIX A – PROJECT SPECIFICATIONS

University of Southern Queensland

FACULTY OF ENGINEERING AND SURVEYING

ENG 4111/4112 Research Project
PROJECT SPECIFICATION

FOR: **MATT PICHLIS**

TOPIC: DEVELOPMENT OF ADVANCED TURBULENT COMBUSTION MODELS

SUPERVISOR: Dr Andrew Wandel

PROJECT AIM: This project aims to further develop the 'Multiple Mapping Conditioning' (MMC) turbulent combustion model and perform a sensitivity test to verify its results.

PROGRAMME: (Issue B, 2 April 2014)

1. Research and study the turbulent combustion model, 'Multiple Mapping Conditioning' (MMC)

2. Investigate the case of a 'Partially Stirred Reactor' (PaSR)

3. Determine appropriate boundary conditions for MMC applied to PaSR

4. Simulate for a wide range of conditions to verify the model

5. Investigate the efficiency and accuracy of different forms of MMC

APPENDIX B – COMPLETE RESULTS

B-1, Simulation with Ren and Pope conditions 1

Simulation was run with the same condition as in B-1 however a different random seed was used to ensure that the results are consistent and the model is can handle the variations.

τres – 2 e-3

τmix – 0.35 τres

[a] – This Plot shows the profile of the reference variable when sorted.

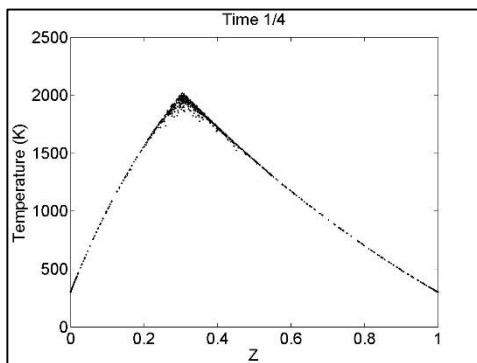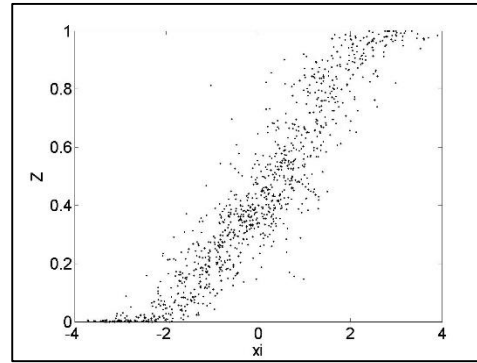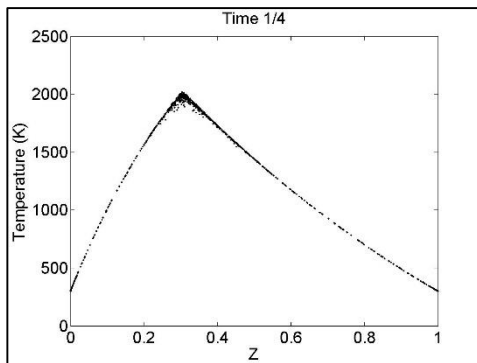[b] – This shows the distribution of the particles in throughout the reference space.

[c,d,e,f] – These plots are taken at time intervals throughout the simulation to demonstrate the behavior of the particles throughout the residence time. Plot f shows the final time step overlaid with the first step to show the total amount of change throughout the simulation.

[a]

[b]

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B-2, Ren and Pope Conditions 2

Simulation was run with the same condition as in B-1 however a different random seed was used to ensure that the results are consistent and the model is can handle the variations.

τres – 2 e-3

τmix – 0.35 τres

[a] – This Plot shows the profile of the reference variable when sorted.

[b] – This shows the distribution of the particles in throughout the reference space.

[c,d,e,f] – These plots are taken at time intervals throughout the simulation to demonstrate the behavior of the particles throughout the residence time. Plot f shows the final time step overlaid with the first step to show the total amount of change throughout the simulation.
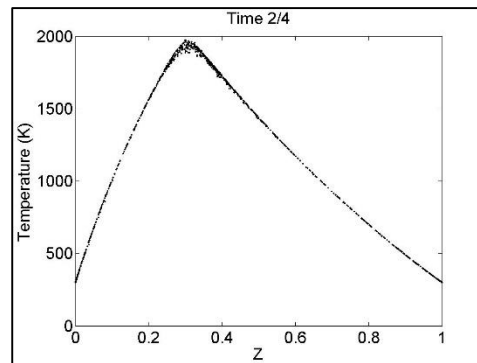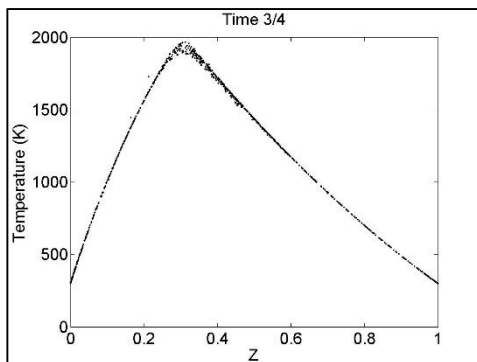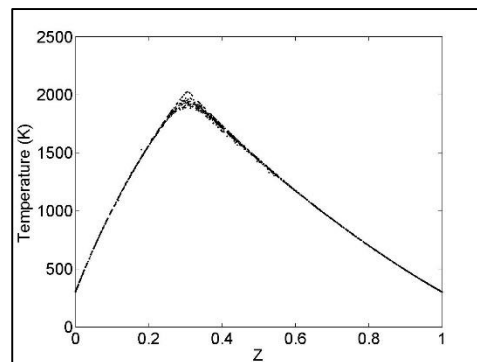

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B-3, Ren and Pope Conditions 3

Simulation was run with the same condition as in B-1 however a different random seed was used to ensure that the results are consistent and the model is can handle the variations.

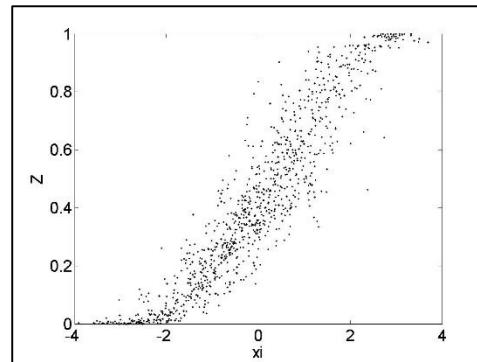τres – 2 e-3

τmix – 0.35 τres

[a] – This Plot shows the profile of the reference variable when sorted.

[b] – This shows the distribution of the particles in throughout the reference space.
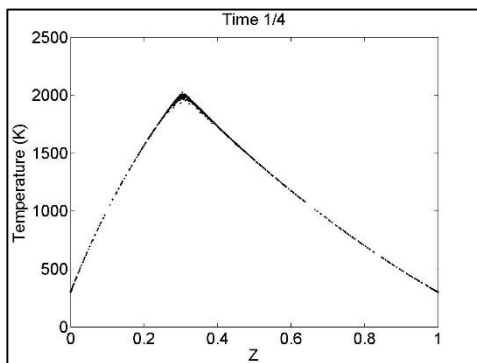
[c,d,e,f] – These plots are taken at time intervals throughout the simulation to demonstrate the behavior of the particles throughout the residence time. Plot f shows the final time step overlaid with the first step to show the total amount of change throughout the simulation.
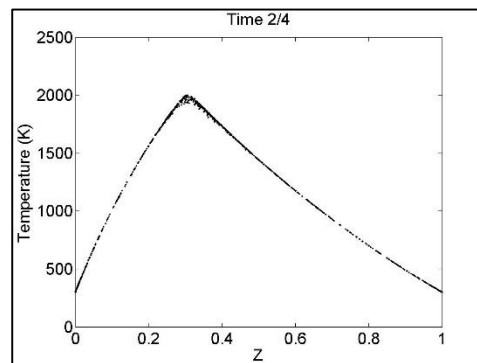
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B-4, Ren and Pope Conditions 4

Simulation was run with the same condition as in B-1 however a different random seed was used to ensure that the results are consistent and the model is can handle the variations.

τres – 2 e-3

τmix – 0.35 τres

[a] – This Plot shows the profile of the reference variable when sorted.

[b] – This shows the distribution of the particles in throughout the reference space.

[c,d,e,f] – These plots are taken at time intervals throughout the simulation to demonstrate the behavior of the particles throughout the residence time. Plot f shows the final time step overlaid with the first step to show the total amount of change throughout the simulation.
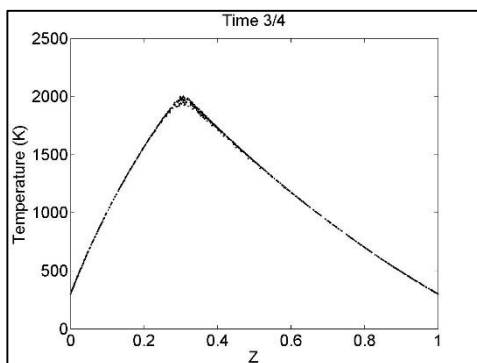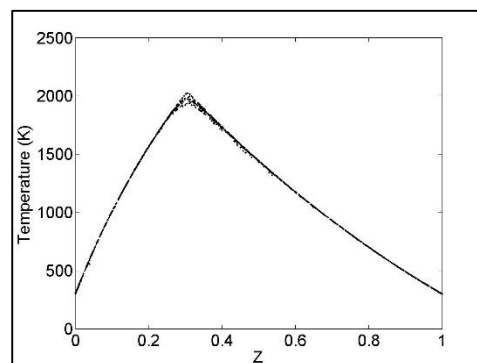

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B-5, Ren and Pope Conditions 5

Simulation was run with the same condition as in B-1 however a different random seed was used to ensure that the results are consistent and the model is can handle the variations.

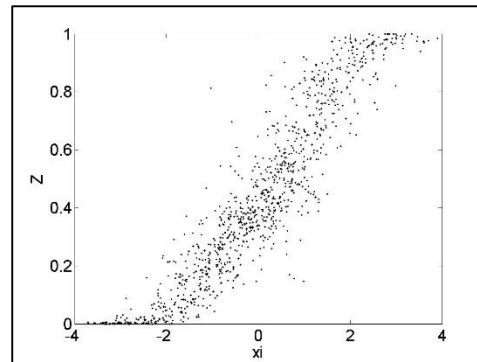τres – 2 e-3

τmix – 0.35 τres

[a] – This Plot shows the profile of the reference variable when sorted.

[b] – This shows the distribution of the particles in throughout the reference space.
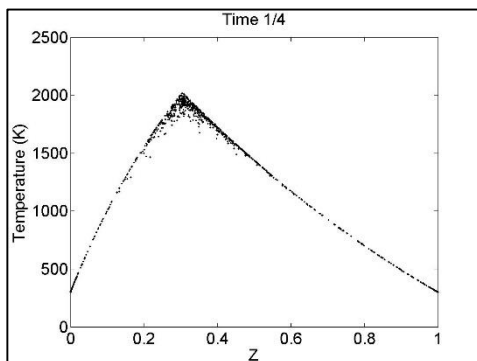
[c,d,e,f] – These plots are taken at time intervals throughout the simulation to demonstrate the behavior of the particles throughout the residence time. Plot f shows the final time step overlaid with the first step to show the total amount of change throughout the simulation.
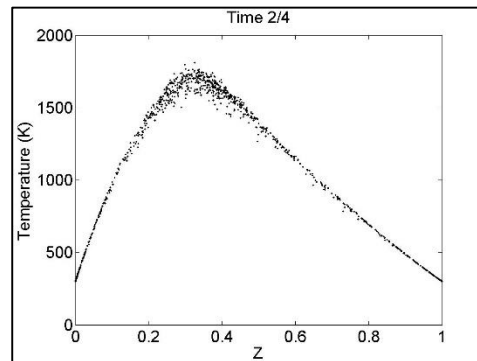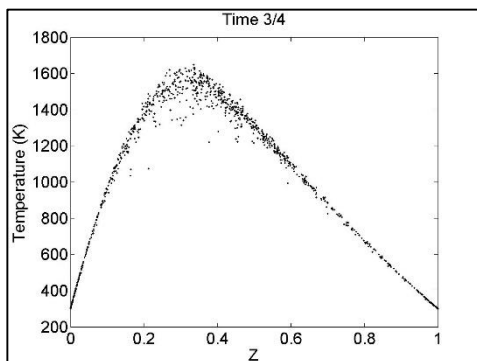

[a]

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B-6, Increased Residence Time Scale 1

Simulation was run with a higher residence time scale with the mixing time scale fraction set as the same fraction of the residence time scale.

τres – 7 e-3

τmix – 0.35 τres

[a] – This Plot shows the profile of the reference variable when sorted.

[b] – This shows the distribution of the particles in throughout the reference space.

[c,d,e,f] – These plots are taken at time intervals throughout the simulation to demonstrate the behavior of the particles throughout the residence time. Plot f shows the final time step overlaid with the first step to show the total amount of change throughout the simulation.
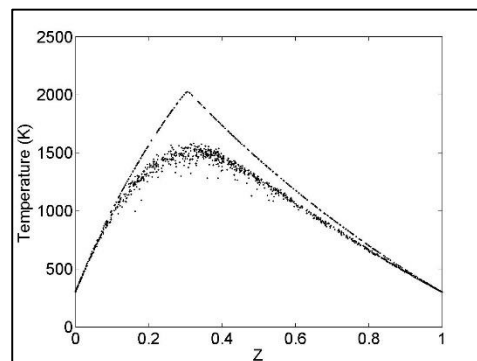

[a]

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B-7, Increased Residence Time Scale 2

Simulation was run with a higher residence time scale with the mixing time scale fraction set as the same fraction of the residence time scale.
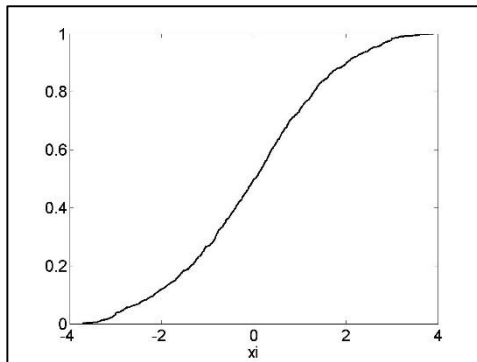
$\tau res - 2$ e-2
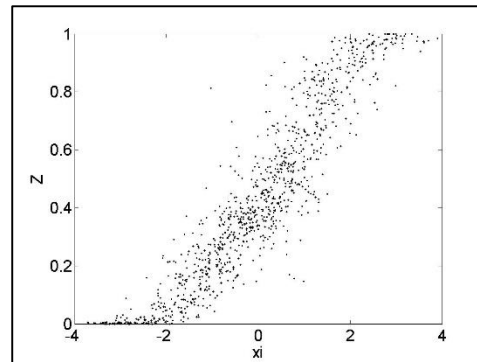
$\tau mix - 0.35$ τres

[a] – This Plot shows the profile of the reference variable when sorted.

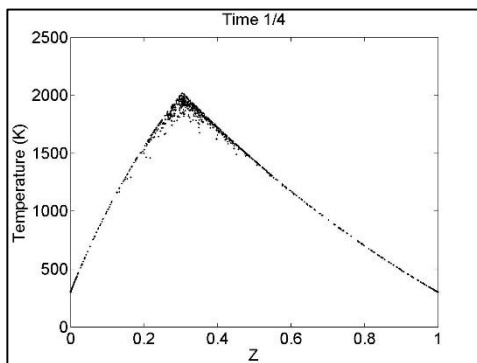[b] – This shows the distribution of the particles in throughout the reference space.

[c,d,e,f] – These plots are taken at time intervals throughout the simulation to demonstrate the behavior of the particles throughout the residence time. Plot f shows the final time step overlaid with the first step to show the total amount of change throughout the simulation.
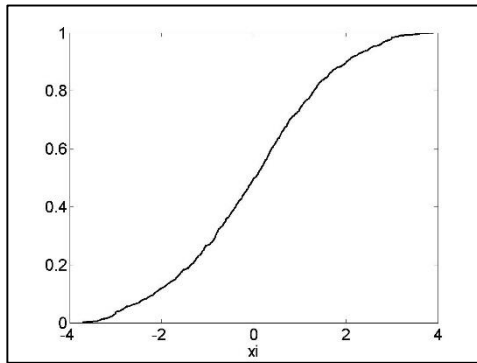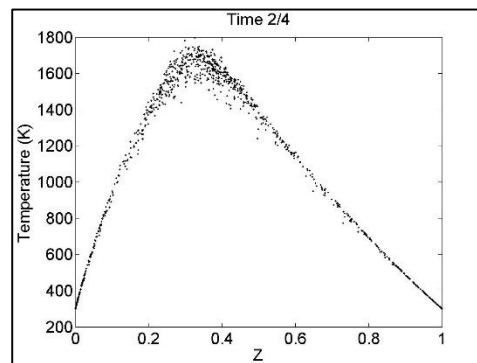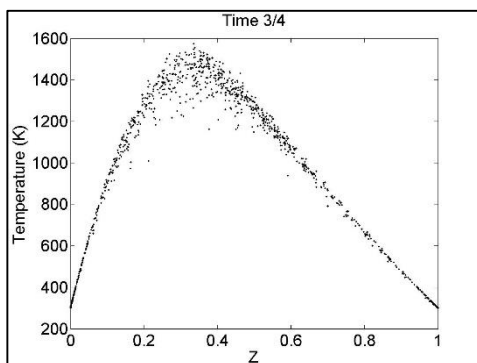
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B-8, Increased Residence Time Scale 3

Simulation was run with a higher residence time scale with the mixing time scale fraction set as the same fraction of the residence time scale.

τres – 7 e-2

τmix – 0.35 τres

[a] – This Plot shows the profile of the reference variable when sorted.

[b] – This shows the distribution of the particles in throughout the reference space.

[c,d,e,f] – These plots are taken at time intervals throughout the simulation to demonstrate the behavior of the particles throughout the residence time. Plot f shows the final time step overlaid with the first step to show the total amount of change throughout the simulation.
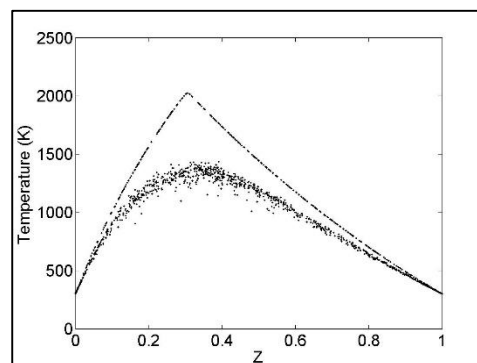
[a]

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B-9, Decreased Residence Time Scale 1

Simulation was run with a lower residence time scale with the mixing time scale fraction set as the same fraction of the residence time scale.
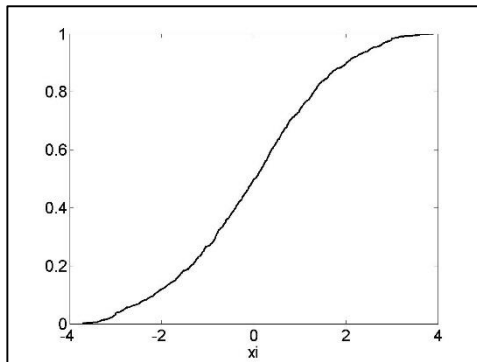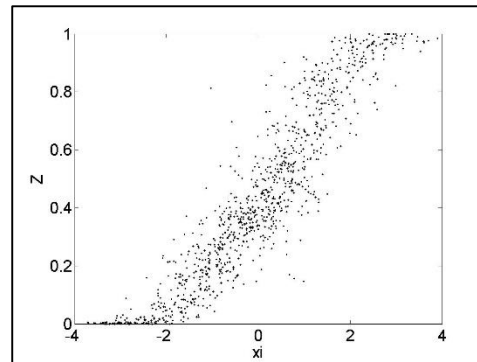
τres – 2 e-4

τmix – 0.35 τres

[a] – This Plot shows the profile of the reference variable when sorted.

[b] – This shows the distribution of the particles in throughout the reference space.
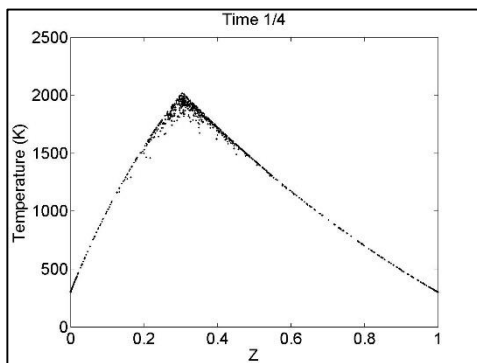
[c,d,e,f] – These plots are taken at time intervals throughout the simulation to demonstrate the behavior of the particles throughout the residence time. Plot f shows the final time step overlaid with the first step to show the total amount of change throughout the simulation.
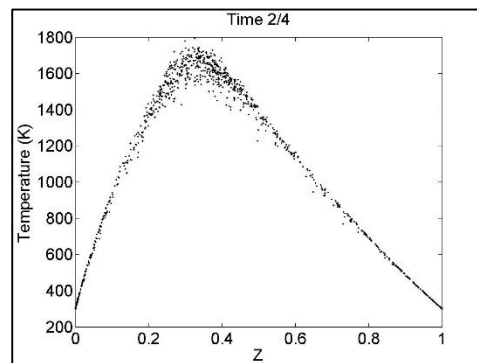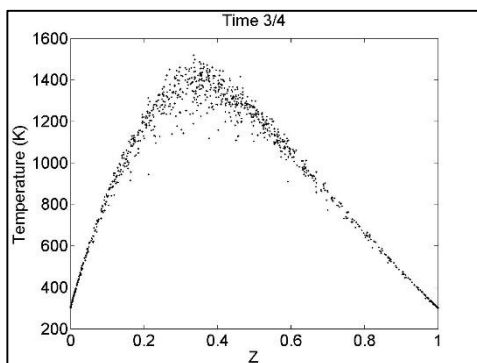

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B-10, Decreased Residence Time Scale 2

Simulation was run with a lower residence time scale with the mixing time scale fraction set as the same fraction of the residence time scale.

τres – 7 e-5

τmix – 0.35 τres

[a] – This Plot shows the profile of the reference variable when sorted.

[b] – This shows the distribution of the particles in throughout the reference space.

[c,d,e,f] – These plots are taken at time intervals throughout the simulation to demonstrate the behavior of the particles throughout the residence time. Plot f shows the final time step overlaid with the first step to show the total amount of change throughout the simulation.
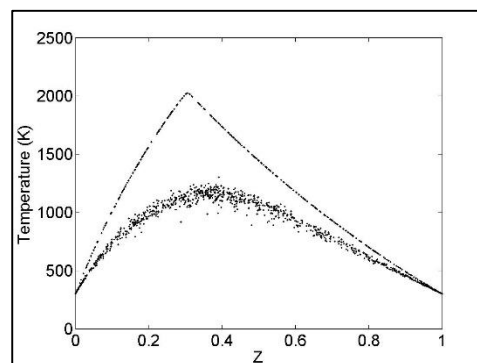

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B-11, Decreased Residence Time Scale 3

Simulation was run with a lower residence time scale with the mixing time scale fraction set as the same fraction of the residence time scale.
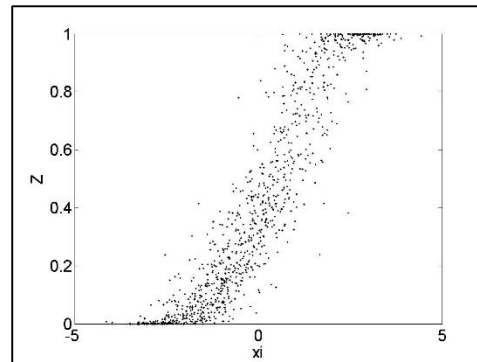
τres – 2 e-5

τmix – 0.35 τres

[a] – This Plot shows the profile of the reference variable when sorted.

[b] – This shows the distribution of the particles in throughout the reference space.
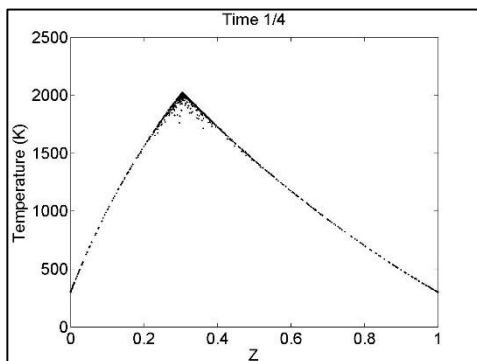
[c,d,e,f] – These plots are taken at time intervals throughout the simulation to demonstrate the behavior of the particles throughout the residence time. Plot f shows the final time step overlaid with the first step to show the total amount of change throughout the simulation.
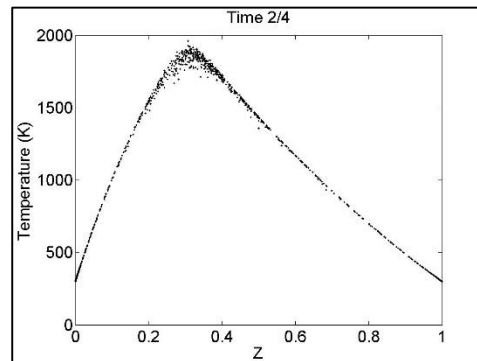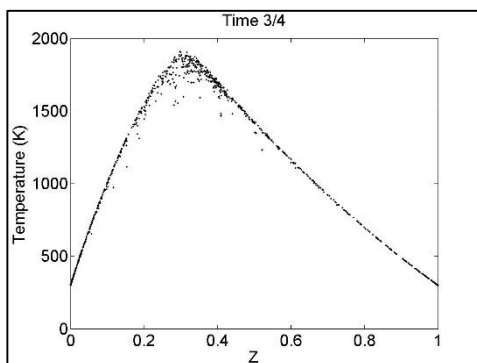

[a]

[b]

[c]

[d]

[e]

[f]

B-12, Increased Mixing Time Scale 1

Simulation was run with an increased mixing time scale and the same residence time scale as the simulations of B1-5.

$\tau res - 2\ e{-}3$

$\tau mix - 0.55\ \tau res$

[a] – This Plot shows the profile of the reference variable when sorted.

[b] – This shows the distribution of the particles in throughout the reference space.

[c,d,e,f] – These plots are taken at time intervals throughout the simulation to demonstrate the behavior of the particles throughout the residence time. Plot f shows the final time step overlaid with the first step to show the total amount of change throughout the simulation.
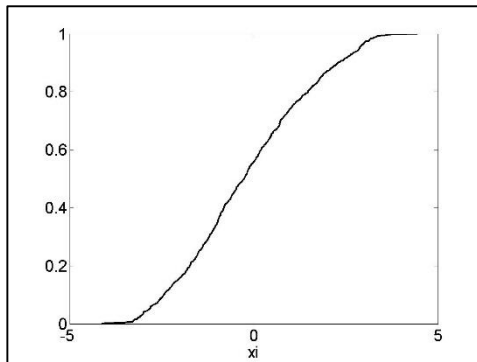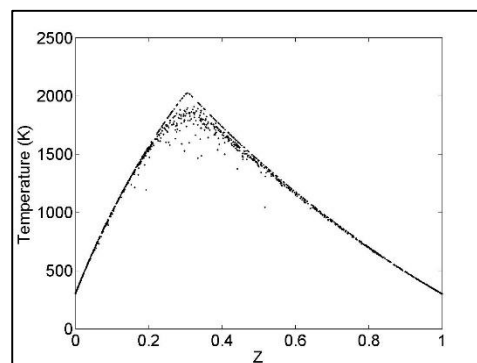

[a]

[b]

[c]

[d]

[e]

[f]

B-13, Increased Mixing Time Scale 2

Simulation was run with an increased mixing time scale and the same residence time scale as the simulations of B1-5.
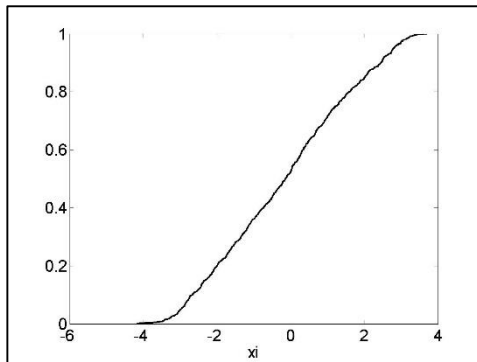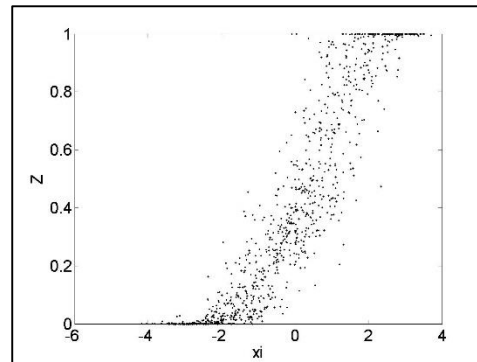
τres – 2 e-3

τmix – 0.75 τres

[a] – This Plot shows the profile of the reference variable when sorted.

[b] – This shows the distribution of the particles in throughout the reference space.
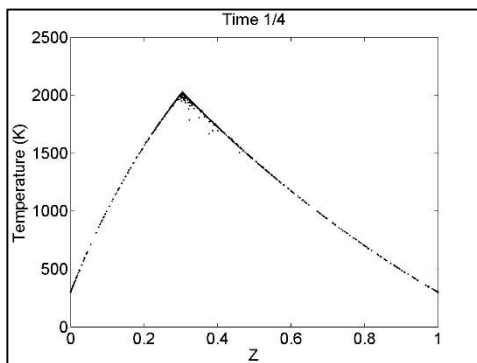
[c,d,e,f] – These plots are taken at time intervals throughout the simulation to demonstrate the behavior of the particles throughout the residence time. Plot f shows the final time step overlaid with the first step to show the total amount of change throughout the simulation.
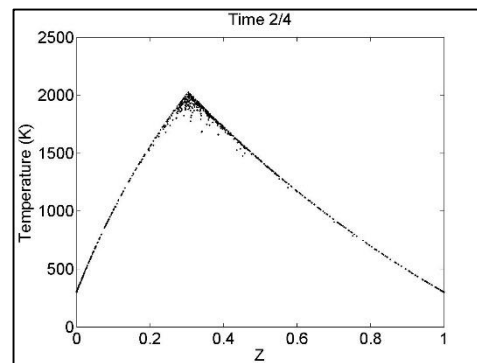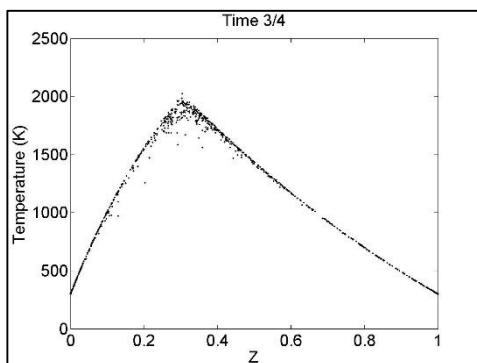

[a]

[b]

[c]

[d]

[e]

[f]

B-14, Increased Mixing Time Scale 3

Simulation was run with an increased mixing time scale and the same residence time scale as the simulations of B1-5.

τres – 2 e-3

τmix – 0.95 τres

[a] – This Plot shows the profile of the reference variable when sorted.

[b] – This shows the distribution of the particles in throughout the reference space.

[c,d,e,f] – These plots are taken at time intervals throughout the simulation to demonstrate the behavior of the particles throughout the residence time. Plot f shows the final time step overlaid with the first step to show the total amount of change throughout the simulation.
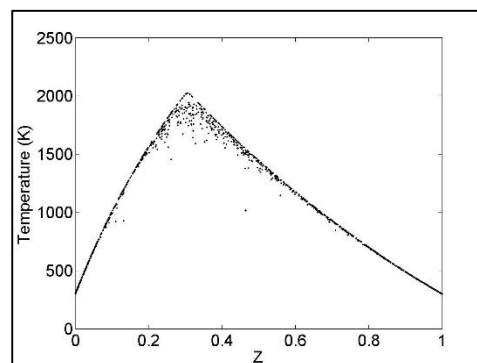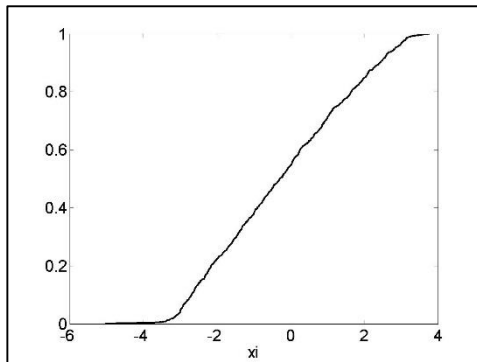

[a]

[b]

[c]

[d]

[e]

[f]

B-15, Decreased Mixing Time Scale 1

Simulation was run with a decreased mixing time scale and the same residence time scale as the simulations of B1-5.
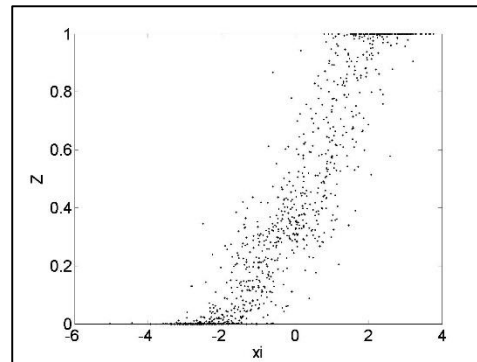
τres – 2 e-3

τmix – 0.25 τres

[a] – This Plot shows the profile of the reference variable when sorted.

[b] – This shows the distribution of the particles in throughout the reference space.
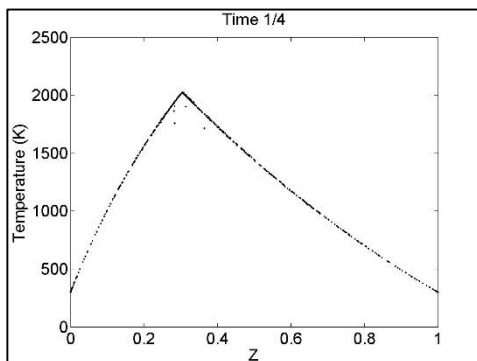
[c,d,e,f] – These plots are taken at time intervals throughout the simulation to demonstrate the behavior of the particles throughout the residence time. Plot f shows the final time step overlaid with the first step to show the total amount of change throughout the simulation.
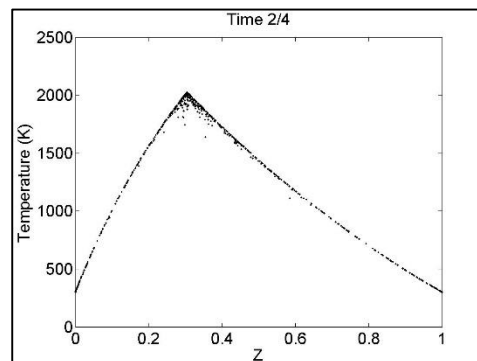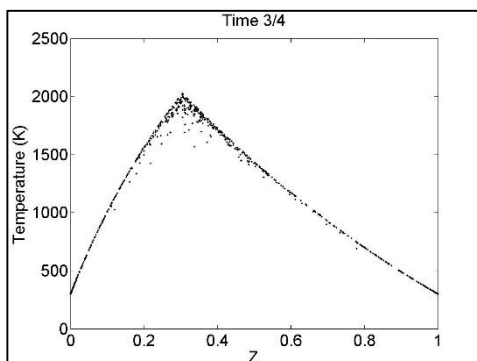

[a]

[b]

[c]

[d]

[e]

[f]

B-16, Decreased Mixing Time Scale 2

Simulation was run with a decreased mixing time scale and the same residence time scale as the simulations of B1-5.

τres – 2 e-3

τmix – 0.15 τres

[a] – This Plot shows the profile of the reference variable when sorted.

[b] – This shows the distribution of the particles in throughout the reference space.

[c,d,e,f] – These plots are taken at time intervals throughout the simulation to demonstrate the behavior of the particles throughout the residence time. Plot f shows the final time step overlaid with the first step to show the total amount of change throughout the simulation.
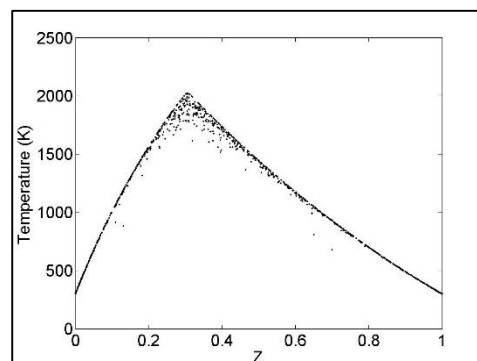

[a]

[b]

[c]

[d]

[e]

[f]

B-17, Decreased Mixing Time Scale 3

Simulation was run with a decreased mixing time scale and the same residence time scale as the simulations of B1-5.
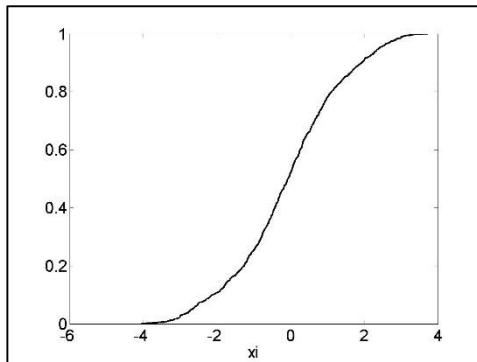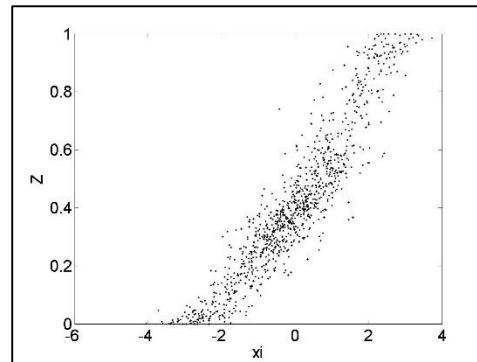
τres – 2 e-3

τmix – 0.05 τres

[a] – This Plot shows the profile of the reference variable when sorted.

[b] – This shows the distribution of the particles in throughout the reference space.
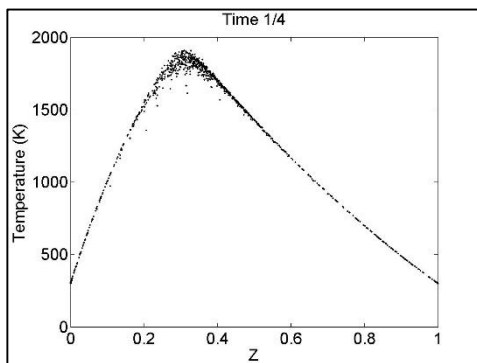
[c,d,e,f] – These plots are taken at time intervals throughout the simulation to demonstrate the behavior of the particles throughout the residence time. Plot f shows the final time step overlaid with the first step to show the total amount of change throughout the simulation.
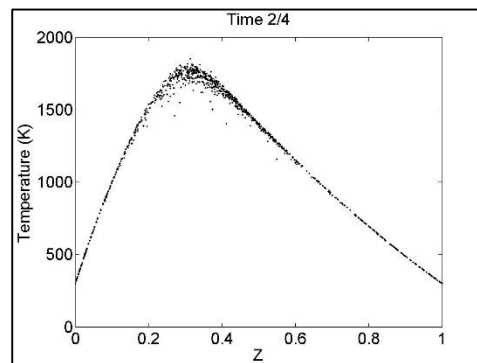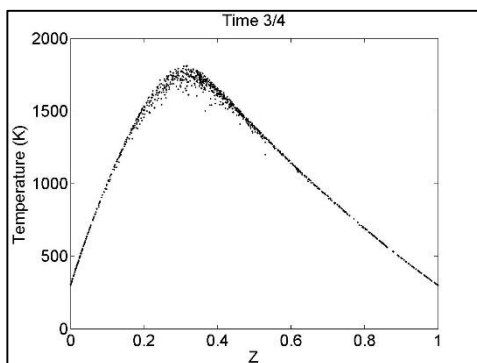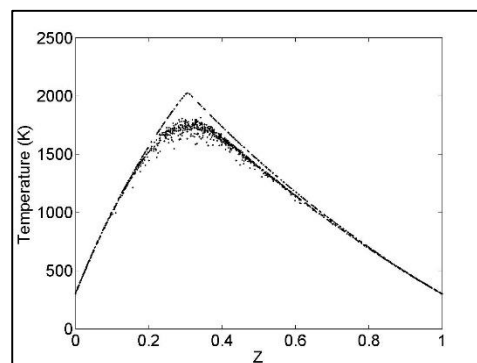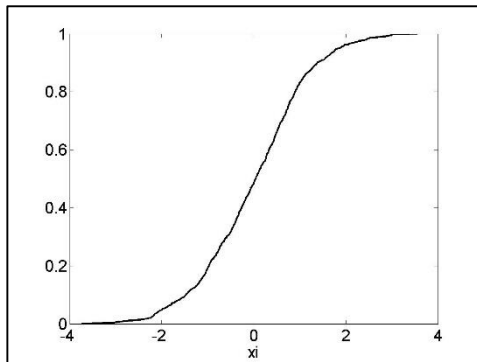

[a]
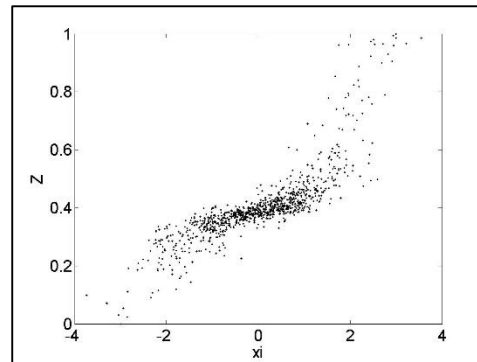
[b]

[c]

[d]

[e]

[f]

APPENDIX C – ALTERED CHEMICAL REACTIONS .CTI FILE

```
#
# Generated from file gri30.inp
# by ck2cti on Mon Aug 25 09:52:57 2003
#
# Modified to H2O2N2 system by Matt Pichlis
# August 2014
#
# Transport data from file ../transport/gri30_tran.dat.

units(length = "cm", time = "s", quantity = "mol",
act_energy = "cal/mol")


ideal_gas(name = "gri30",
      elements = " O  H  N ",
      species = """ H2  H  O  O2  OH  H2O  HO2  H2O2
N2 """,
      reactions = "all",
      initial_state = state(temperature = 300.0,
                        pressure = OneAtm)    )

ideal_gas(name = "gri30_mix",
      elements = " O  H  N ",
      species = """ H2  H  O  O2  OH  H2O  HO2  H2O2
N2 """,
      reactions = "all",
      transport = "Mix",
      initial_state = state(temperature = 300.0,
                        pressure = OneAtm)    )


ideal_gas(name = "gri30_multi",
      elements = " O  H  N ",
      species = """ H2  H  O  O2  OH  H2O  HO2  H2O2
N2 """,
      reactions = "all",
      transport = "Multi",
      initial_state = state(temperature = 300.0,
                        pressure = OneAtm)    )




#-------------------------------------------------------
-----------------------
#  Species data
#-------------------------------------------------------
-----------------------

species(name = "H2",
    atoms = " H:2 ",
    thermo = (
        NASA( [  200.00,  1000.00], [  2.344331120E+00,
7.980520750E-03,
                -1.947815100E-05,   2.015720940E-08,  -
7.376117610E-12,
                -9.179351730E+02,   6.830102380E-01] ),
```
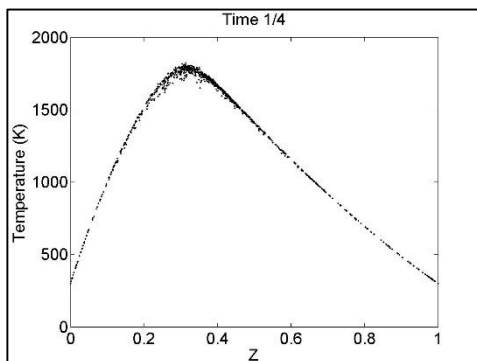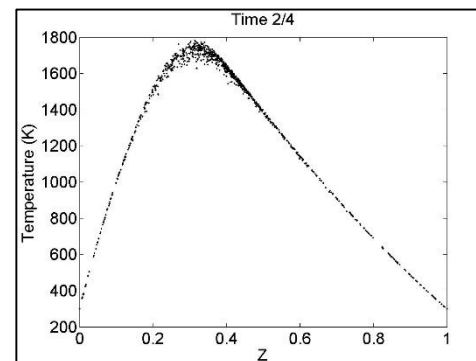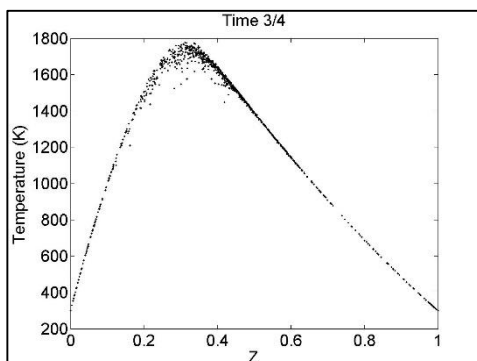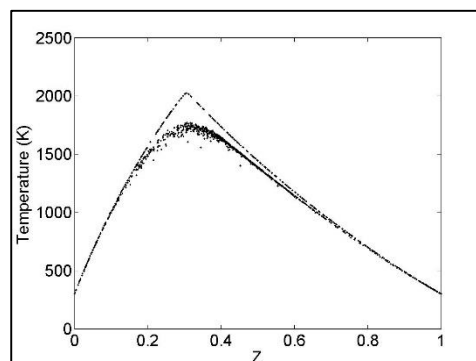
```
          NASA( [ 1000.00,  3500.00], [  3.337279200E+00,
-4.940247310E-05,
                4.994567780E-07,  -1.795663940E-10,
2.002553760E-14,
                -9.501589220E+02,  -3.205023310E+00] )
            ),
    transport = gas_transport(
                    geom = "linear",
                    diam =     2.92,
                    well_depth =    38.00,
                    polar =     0.79,
                    rot_relax =   280.00),
    note = "TPIS78"
       )

species(name = "H",
    atoms = " H:1 ",
    thermo = (
       NASA( [  200.00,  1000.00], [  2.500000000E+00,
7.053328190E-13,
                -1.995919640E-15,   2.300816320E-18,  -
9.277323320E-22,
                2.547365990E+04,  -4.466828530E-01] ),
       NASA( [ 1000.00,  3500.00], [  2.500000010E+00,
-2.308429730E-11,
                1.615619480E-14,  -4.735152350E-18,
4.981973570E-22,
                2.547365990E+04,  -4.466829140E-01] )
            ),
    transport = gas_transport(
                    geom = "atom",
                    diam =     2.05,
                    well_depth =   145.00),
    note = "L 7/88"
       )

species(name = "O",
    atoms = " O:1 ",
    thermo = (
       NASA( [  200.00,  1000.00], [  3.168267100E+00,
-3.279318840E-03,
                6.643063960E-06,  -6.128066240E-09,
2.112659710E-12,
                2.912225920E+04,   2.051933460E+00] ),
       NASA( [ 1000.00,  3500.00], [  2.569420780E+00,
-8.597411370E-05,
                4.194845890E-08,  -1.001777990E-11,
1.228336910E-15,
                2.921757910E+04,   4.784338640E+00] )
            ),
    transport = gas_transport(
                    geom = "atom",
                    diam =     2.75,
                    well_depth =    80.00),
    note = "L 1/90"
       )
```

```
species(name = "O2",
    atoms = " O:2 ",
    thermo = (
       NASA( [  200.00,  1000.00], [  3.782456360E+00,
-2.996734160E-03,
                9.847302010E-06,  -9.681295090E-09,
3.243728370E-12,
                -1.063943560E+03,   3.657675730E+00] ),
       NASA( [ 1000.00,  3500.00], [  3.282537840E+00,
1.483087540E-03,
                -7.579666690E-07,   2.094705550E-10,  -
2.167177940E-14,
                -1.088457720E+03,   5.453231290E+00] )
            ),
    transport = gas_transport(
                    geom = "linear",
                    diam =     3.46,
                    well_depth =   107.40,
                    polar =     1.60,
                    rot_relax =     3.80),
    note = "TPIS89"
       )

species(name = "OH",
    atoms = " O:1  H:1 ",
    thermo = (
       NASA( [  200.00,  1000.00], [  3.992015430E+00,
-2.401317520E-03,
                4.617938410E-06,  -3.881133330E-09,
1.364114700E-12,
                3.615080560E+03,  -1.039254580E-01] ),
       NASA( [ 1000.00,  3500.00], [  3.092887670E+00,
5.484297160E-04,
                1.265052280E-07,  -8.794615560E-11,
1.174123760E-14,
                3.858657000E+03,   4.476696100E+00] )
            ),
    transport = gas_transport(
                    geom = "linear",
                    diam =     2.75,
                    well_depth =    80.00),
    note = "RUS 78"
       )

species(name = "H2O",
    atoms = " H:2  O:1 ",
    thermo = (
       NASA( [  200.00,  1000.00], [  4.198640560E+00,
-2.036434100E-03,
                6.520402110E-06,  -5.487970620E-09,
1.771978170E-12,
                -3.029372670E+04,  -8.490322080E-01] ),
       NASA( [ 1000.00,  3500.00], [  3.033992490E+00,
2.176918040E-03,
```

```
                            -1.640725180E-07,  -9.704198700E-11,
1.682009920E-14,
                            -3.000429710E+04,   4.966770100E+00] )
                ),
    transport = gas_transport(
                    geom = "nonlinear",
                    diam =      2.60,
                    well_depth =   572.40,
                    dipole =     1.84,
                    rot_relax =      4.00),
    note = "L 8/89"
        )

species(name = "HO2",
    atoms = " H:1  O:2 ",
    thermo = (
        NASA( [  200.00,  1000.00], [  4.301798010E+00,
-4.749120510E-03,
                2.115828910E-05,  -2.427638940E-08,
9.292251240E-12,
                2.948080400E+02,   3.716662450E+00] ),
        NASA( [ 1000.00,  3500.00], [  4.017210900E+00,
2.239820130E-03,
                -6.336581500E-07,   1.142463700E-10,  -
1.079085350E-14,
                1.118567130E+02,   3.785102150E+00] )
                ),
    transport = gas_transport(
                    geom = "nonlinear",
                    diam =      3.46,
                    well_depth =   107.40,
                    rot_relax =      1.00),
    note = "L 5/89"
        )

species(name = "H2O2",
    atoms = " H:2  O:2 ",
    thermo = (
        NASA( [  200.00,  1000.00], [  4.276112690E+00,
-5.428224170E-04,
                1.673357010E-05,  -2.157708130E-08,
8.624543630E-12,
                -1.770258210E+04,   3.435050740E+00] ),
        NASA( [ 1000.00,  3500.00], [  4.165002850E+00,
4.908316940E-03,
                -1.901392250E-06,   3.711859860E-10,  -
2.879083050E-14,
                -1.786178770E+04,   2.916156620E+00] )
                ),
    transport = gas_transport(
                    geom = "nonlinear",
                    diam =      3.46,
                    well_depth =   107.40,
                    rot_relax =      3.80),
    note = "L 7/88"
        )
```

```
species(name = "N2",
    atoms = " N:2 ",
    thermo = (
       NASA( [  300.00,  1000.00], [  3.298677000E+00,
1.408240400E-03,
              -3.963222000E-06,   5.641515000E-09,   -
2.444854000E-12,
              -1.020899900E+03,   3.950372000E+00] ),
       NASA( [ 1000.00,  5000.00], [  2.926640000E+00,
1.487976800E-03,
              -5.684760000E-07,   1.009703800E-10,   -
6.753351000E-15,
              -9.227977000E+02,   5.980528000E+00] )
           ),
    transport = gas_transport(
                   geom = "linear",
                   diam =      3.62,
                   well_depth =     97.53,
                   polar =     1.76,
                   rot_relax =      4.00),
    note = "121286"
       )


#-------------------------------------------------------
-----------------------
#  Reaction data
#-------------------------------------------------------
-----------------------

#  Reaction 1
reaction( "O2 + H <=> OH + O",    [2.00000E+14, 0,
16802.1])

#  Reaction 2
reaction( "H2 + O <=> OH + H",    [5.06000E+04, 2.7,
6285.851])

#  Reaction 3
reaction( "H2 + OH <=> H2O + H",    [1.00000E+08, 1.6,
3298.279])

#  Reaction 4
reaction( "OH + OH <=> H2O + O",    [1.50000E+09, 1.1,
95.60229])

#  Reaction 5
three_body_reaction( "H + H + M <=> H2 + M",
[1.80000E+18, -1, 0])

#  Reaction 6
three_body_reaction( "H + OH + M <=> H2O + M",
[2.20000E+22, -2, 0])

#  Reaction 7
```

```
three_body_reaction( "O + O + M <=> O2 + M",
[2.90000E+17, -1, 0])

#   Reaction 8
three_body_reaction( "H + O2 + M <=> HO2 + M",
[2.30000E+18, -0.8, 0])

#   Reaction 9
reaction( "HO2 + H <=> OH + OH",    [1.50000E+14, 0,
1003.824])

#   Reaction 10
reaction( "HO2 + H <=> H2 + O2",    [2.50000E+13, 0,
693.1166])

#   Reaction 11
reaction( "HO2 + H <=> H2O + O",    [3.00000E+13, 0,
1720.841])

#   Reaction 12
reaction( "HO2 + O <=> OH + O2",    [1.80000E+13, 0, -
406.31])

#   Reaction 13
reaction( "HO2 + OH <=> H2O + O2",    [6.00000E+13, 0,
0])

#   Reaction 14
reaction( "HO2 + HO2 => H2O2 + O2",    [2.50000E+11, 0,
-1242.83])

#   Reaction 15
three_body_reaction( "OH + OH + M <=> H2O2 + M",
[3.25000E+22, -2, 0])

#   Reaction 16
reaction( "H2O2 + H <=> H2 + HO2",    [1.70000E+12, 0,
3752.39])

#   Reaction 17
reaction( "H2O2 + H <=> H2O + OH",    [1.00000E+13, 0,
3585.086])

#   Reaction 18
reaction( "H2O2 + O <=> OH + HO2",    [2.80000E+13, 0,
6405.354])

#   Reaction 19
reaction( "H2O2 + OH <=> H2O + HO2",    [5.40000E+12, 0,
1003.824])
```