UNSUPERVISED CLUSTERING: A MIXTURE OF EXPERTS FRAMEWORK TO REPRESENT FLAMELET TABLES

An Undergraduate Research Scholars Thesis

by

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Submitted to the LAUNCH: Undergraduate Research office at
Texas A&M University
in partial fulfillment of the requirements for the designation as an

UNDERGRADUATE RESEARCH SCHOLAR

Approved by
Faculty Research Advisor: Dr. Dorrin Jarrahbashi

May 2022

Major: Mechanical Engineering

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ABSTRACT

Unsupervised Clustering: A Mixture of Experts Framework to Represent Flamelet Tables

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A novel unsupervised learning-based clustering approach to represent the flamelet tables is developed. The typical tabulation method for flamelet-based modeling generally requires a large amount of storage. A well-developed machine learning model can accurately represent flamelet tables while taking up significantly less storage. The proposed method utilizes a mixture of experts (MoE) technique where specialized Deep Neural Networks (DNNs) are trained on different parts of the input space. This identification of combustion manifolds within the input space is accomplished through the use of an unsupervised learning-based clustering algorithm, which is able to categorize an input to a specific cluster. Previous studies have shown that developing specialized models can lead to a higher accuracy and faster access to the flamelet tables. However, the clustering techniques utilized in these studies do not investigate an unsupervised learning approach. The proposed model is trained and evaluated on 5-dimensional flamelet tables, and an investigation of clustering techniques and optimal number of clusters is also conducted. This research project shows that unsupervised learning-based clustering algorithms coupled with a MoE framework of DNNs can accurately predict temperatures and mass fractions in flamelet tables.

ACKNOWLEDGMENTS

Contributors

I would like to thank my faculty advisor, Dr. Jarrahbashi, and my graduate student research advisor, Rohit Mishra, for their guidance and support throughout the course of this research.

Additionally, thanks to my family and friends for their constant encouragement and support.

Portions of this research were conducted with the advanced computing resources provided by Texas A&M High Performance Research Computing.

All other work conducted for the thesis was completed by the student independently.

Funding Sources

This undergraduate research was not supported by any contributors or funding.

NOMENCLATURE

Z	Mixture fraction
$\tilde{Z''^2}$	Mixture fraction variance
χ	Scalar dissipation rate
χ_{st}	Stoichiometric scalar dissipation rate
λ/Λ	Reaction progress parameter
$\tilde{\phi}/\psi$	Thermo-chemical scalars (Mass fractions or Temperature)
β	Beta function
χ_q	Scalar dissipation rate at quenching
C	Reaction progress variable

1. INTRODUCTION

Combustion simulation is important because it allows for the analysis of flow and reactions that occur during combustion. A well-developed, accurate simulation can help reduce pollutant formation and increase efficiency. This typically involves the calculation of relevant information such as temperature and mass fractions of certain compounds that are present.

Combustion modeling has improved significantly in recent years due to advancements in computational resources and numerical algorithms. However, this field is not fully understood because of two complex processes and their interaction: turbulence and chemistry.

1.1 Combustion Modeling

Significant advancements in modeling turbulence have resulted in trade-off models that can be seamlessly applied to engineering applications using Large Eddy Simulation (LES). This type of modeling takes less computational time compared to Direct Numerical Simulation (DNS), but is more accurate than Reynolds-Averaged Navier Stokes (RANS). Zero and one equation forms of LES modeling have been explored in relation to their application to combustion, but it continues to be a topic of further research [1].

On the chemistry front, major efforts in the literature have been dedicated towards reducing the chemistry or representing it in such a way that minimum loss of information is ensured. Since solving the stiff ordinary differential equations (ODEs) individually for each species' mass fraction becomes computationally prohibitive, this type of reduction becomes a necessity for all practical engineering applications.

Two ways of treating chemistry include reduction of chemical kinetic mechanisms and *a priori* 1-Dimensional tabulations. The former has been developed over time with schemes such as Directed Relation Graphs (DRG) [2], Directed Relation Graphs with Error Propagation (DRGEP) [3], Dynamic Adaptive Chemistry (DAC) [4], Path Flux Analysis (PFA) [5], Global Pathway Selection (GPS) [6], etc. A combination of these two methods, Tabulated Dynamic Adaptive Chemistry

(TDAC) [7], is made of DAC [4] and In-Situ Adaptive Tabulation (ISAT) [8], and has been widely used in the combustion community. The latter also has multiple forms and is mainly called the "flamelet approach".

A flamelet is defined as thin reactive-diffusive layers embedded within an otherwise non-reacting turbulent flow field. In the flamelet modeling approach, the turbulent diffusion flame (**Figure 1.1**) is treated as an ensemble of stretched laminar flamelets [9]. The principle behind the flamelet approach is to only solve the important scalars and find statistical moments of the mass fractions and temperature which relates to these scalars through flamelet equations.

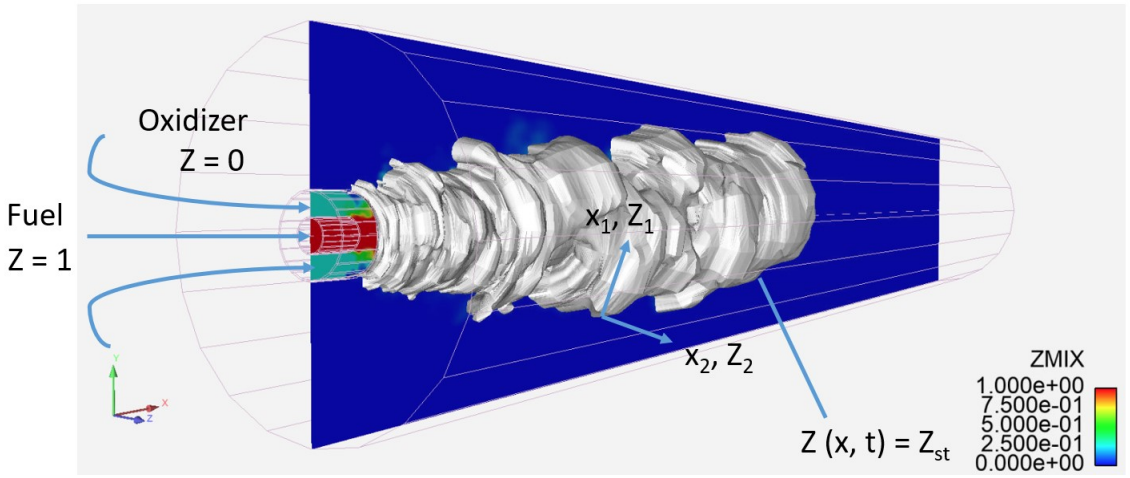

Figure 1.1: Schematic of the surface of stoichiometric mixture in a turbulent jet diffusion flame (Sandia Flame D [10] modeled in NGA [11])

1.2 Flamelet Approaches

Multiple forms of the flamelet approaches presented in the literature are listed as follows:

1.2.1 Steady Laminar Flamelet Model (SLM) [9] [12]

This model was developed for non-premixed combustion with the assumption that the chemical time scales are short enough such that the reactions occur in a thin layer around the stoichiometric mixture at a scale smaller than the eddies. This leads to a local reaction zone which

is laminar, while the diffusion occurs in the direction normal to surface of stoichiometric mixture as shown in **Figure 1.1**.

$$\tilde{\phi} = \int_0^1 \phi(Z, \chi_{st})\beta(Z; \tilde{Z}, \tilde{Z''^2})dZ \qquad \text{(Eq. 1)}$$

Eq. 1 represents the scalar quantity ($\tilde{\phi}$) (mass fractions or temperature) in terms of $\tilde{Z}$, $\tilde{Z''^2}$, and χ_{st}.

1.2.2 Flamelet Progress Variable (FPV) [13] [14]

The SLM model is easy to implement and works well within the framework of the above-mentioned assumptions. However, one of the major drawbacks of the SLM model is its inability to predict the flame lift-off location. Additionally, the SLM model cannot describe the local extinction and re-ignition events properly. The SLM model predicts the upper and lower branches of the S-curve represented in **Figure 1.2**, but leads to numerical instabilities while predicting the middle branch. Therefore, having only the upper and lower branch can lead to large jumps in temperature and density for dissipation rates around the extinction limit. Pierce et al. [13] suggested an improvement over the SLM model. Instead of using the scalar dissipation rate, the model represents the scalar quantities based on two parameters, namely mixture fraction Z and reaction progress parameter λ (Eq. 2). The biggest advantage of switching to the reaction progress parameter is that it better describes local extinction and re-ignition

$$\tilde{\phi} = \int_0^1 \phi(Z, \lambda)\beta(Z; \tilde{Z}, \tilde{Z''^2})dZ \qquad \text{(Eq. 2)}$$

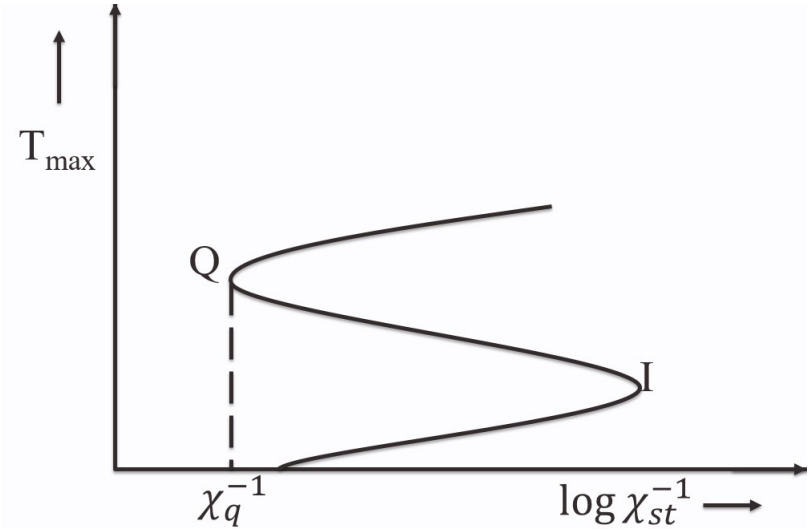

Figure 1.2: S-shaped curve showing quenching (Q) and auto-ignition (I).

Ihme et al. [14] developed conditional PDFs of λ using beta and delta distribution conditioned on Z. They showed that while the delta function overpredicted the mean temperature with moderate extinction, the beta function was able to capture extinction and re-ignition with mean temperature matching DNS data. However, inaccuracies were seen in regions $Z = Z_{st}$ owing to the unsteadiness in those regions. Flamelet Generated Manifold (FGM) [15] is a similar approach to FPV, however, it differs in the way the unsteady branch is accounted for. While the FPV approach solves flamelet equations for middle and lower branches on the S-curve, FGM considers an unsteady extinguishing flamelet.

1.2.3 Unsteady Flamelet [9] [16]

Although the above models are able to predict the mass fractions of major species and heat release accurately, slow chemical processes (e.g. formation of nitric oxide (NO)) require consideration of unsteady effects. The two reasons for the inability of the steady flamelet models to predict slow processes are: strong decay of scalar dissipation rate along the jet axis and radiative heat losses. Peters et al. [9] and Pitsch et al. [16] calculated the unsteady flamelet as a function of the flamelet time (Eq. 3) which is related to the distance from the nozzle.

$$t = \int_0^x \frac{1}{u(x')|(\tilde{Z} = Z_{st})} \phi(Z, \lambda)\beta(Z; \tilde{Z}, \tilde{Z''^2})dx' \qquad \text{(Eq. 3)}$$

Using this type of unsteady treatment, the study [16] was able to predict the axial and radial profiles of NO accurately. On the other hand, the steady flamelet was off by an order of magnitude. Ihme et al. [17] made a time-scale independent formulation of UFPV (Eq. 4) by characterizing the transient flame by mixture fraction, reaction progress variable, and scalar dissipation rate. The flame structure is then obtained from the unsteady flamelet equations.

$$\psi = F_{\psi}^{U}(Z, \Lambda, \chi_{Z,st}) \qquad \text{(Eq. 4)}$$

Bajaj et al. [18] showed that the above formulation can be implemented to predict the auto-ignition and flame lift-off location for n-heptane jets over a broad range of conditions.

1.3 Neural Network Representation

The flamelet tables have proved to be very useful in capturing the chemistry and reducing the computational time. However, these multi-dimensional tables require huge amounts of storage to get accurate chemistry representation; especially, near the extinction-re-ignition zone. To overcome this problem, artificial neural networks (ANNs) have been used in the past to train the model to represent the multi-dimensional dataset. Some of the past studies in this field are conducted by Ihme et al.[19], Emami et al. [20], Owoyele et al. [21], and Ranade et al. [22] among others. Ranade et al. [22] listed the drawbacks of the ANN approach as follows:

1. Training dataset with possibly millions of points over multiple scalars becomes very computationally expensive for large number of species.

2. The nonlinear mathematical functions can be two orders of magnitudes more expensive to compute than linear interpolations.

3. Model training becomes formidable for some important combustion species such as OH and NOx as they require elaborate networks which can affect the overall accuracy and computa-

tional costs.

4. An added layer of complexity can be due to the non-adiabatic nature of the problem.

Apart from the above drawbacks, one additional complexity arises from integrating an ANN with the UFPV approach which adds to the complexity of the multi-dimensional table.

Ranade et al. [22] used an unsupervised dimensionality reduction technique called self-organizing maps (SOM) to reduce the dimension of the table and cluster the different manifolds in the table. However, the data was used to train all the clusters and not just the ones that were selected by SOM. So far, the machine learning implementations have been designed and implemented on FPV type of flamelets.

Owoyele et al. [23] created a mixture of experts (MoE) type of framework which worked on the multidimensional UFPV tables. They showed how their approach predicted the thermo-chemical scalars with higher accuracy as compared to the single neural network (SNN). In contrast to the previous work [23], this research implements unsupervised learning-based clustering algorithms, which have not been well documented with regards to flamelet based modeling. Clustering techniques have been explored with regards to partitioning the composition space during adaptive reduced chemistry [24]. However, the use of unsupervised learning-based clustering algorithms has not been well explored, especially in an advanced MoE framework. Since the data is made up of multiple inter-dependent variables, the existing MoE framework [23] can be optimized using a supervised gating network for a given set of data. However, to make this type of framework work for any data with varying inlet conditions, data-sizes, and unknown manifolds, an unsupervised network seems to be an ideal choice. In this paper the various unsupervised learning-based gating networks applied to an MoE framework are discussed and the importance of optimizing the number of clusters and the clustering technique is established.

2. METHODS

First, the generated flamelet table is described, followed by an explanation of the model architecture and its implementation.

2.1 Dataset

The dataset used to develop the model presented in this study was generated using FlameMaster software [25] with the GRI-Mech 3.0 [26] chemical kinetic mechanism. This is an optimized mechanism designed to provide basic chemical kinetics in combination with modeling of various combustion properties. The generated data models non-premixed combustion of methane (CH_4) as fuel and air as oxidizer using 28 species and 325 reactions. The Arc Continuation method was used to generate the flamelet tables indicating the FPV model used. The initial conditions are: 1 bar pressure and temperature of 300 Kelvin. Flamelets are counterflow diffusion in mixture fraction space with variable scalar dissipation rate.

A flamelet table was generated using inputs of stoichiometric scalar dissipation rate (χ_{st}) and mixture fraction (Z). In total, 59 χ_{st} values were used ranging in values from 0 to 31, and 1003 Z values were used ranging from 0 to 1. This ultimately leads to a total dataset size of 59,177. All the values were normalized to ensure the model would not be dealing with extremely different ranges of values. The figure below (**Figure 2.1**) shows the generated OH mixture fraction data with respect to the inputs χ_{st} and Z. When $Z = Z_{st}$, stoichiometric combustion occurs and the maximum heat release and OH production occurs. At other values of Z, the fuel oxidizer mixture is off balance, which means the combustion is not sustained and the OH mass fraction is low. Additionally, there is an optimal χ_{st} value with the highest OH mass fraction that is most favorable for combustion. A χ_{st} value that is too high will result in quenching of the flame due to heat loss and a low scalar dissipation will cause the fuel and oxidizer to not mix enough.

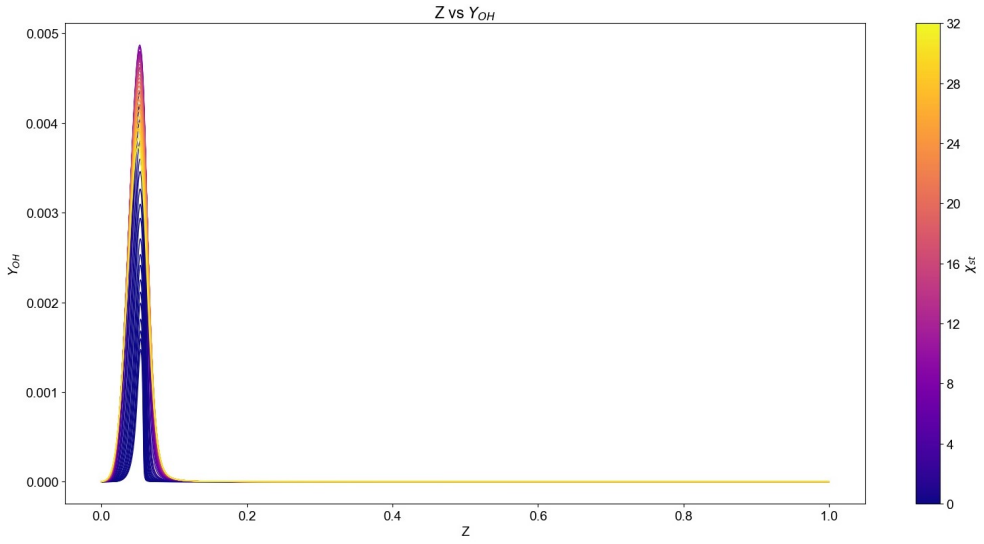

Figure 2.1: Y_{OH} data from generated flamelet table.

2.2 Model Architecture

The model structure used in this research is shown in **Figure 2.2**, which follows a similar MoE approach to that used by Owoyele et al. [23]. A gating network takes in defined inputs and assigns the query to the appropriate expert model. These expert models are Deep Neural Networks (DNNs) that have been trained on specific portions of the dataset. The expert models then take in the corresponding inputs and makes a prediction for the value of interest (temperature, Y_{OH}, etc.).

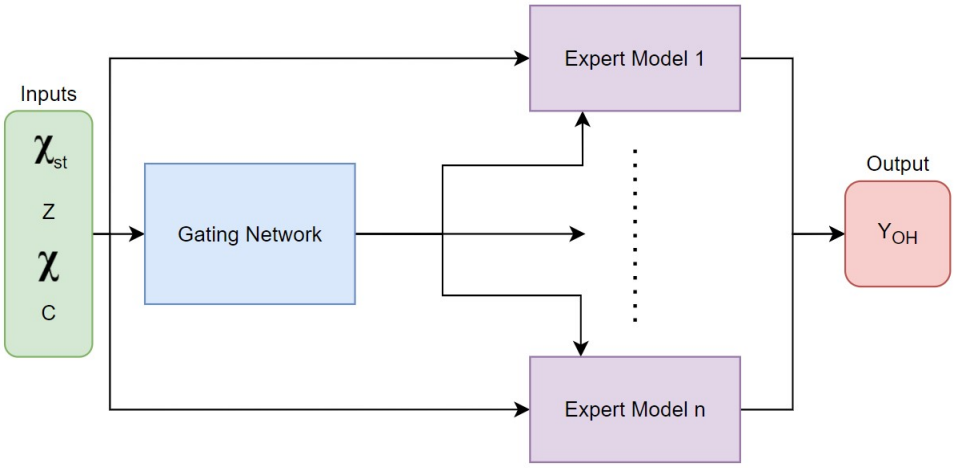

Figure 2.2: Model structure for Y_{OH} prediction.

In order to construct the gating network, the various clusters must first be defined. Clustering of the input space is critical to the performance and evaluation of the proposed model. It has been determined that the flamelet table input space can be divided into manifolds that display different behavior. However, the locations of these manifolds have not been well defined. The purpose of the clustering algorithm is to define the locations of these clusters and determine how the input space is subdivided. Although a dimensionality reduction and clustering technique was tested by Ranade et al. [22], a more advanced architecture is presented here which trains only the corresponding expert model on a given clustered dataset instead of training all the experts as was done in their study. The clustering algorithms evaluated in this research are part of the Sci-Kit Learn library [27], including K-Means Clustering and Gaussian Mixture Model. The number of clusters must be pre-defined for these clustering algorithms.

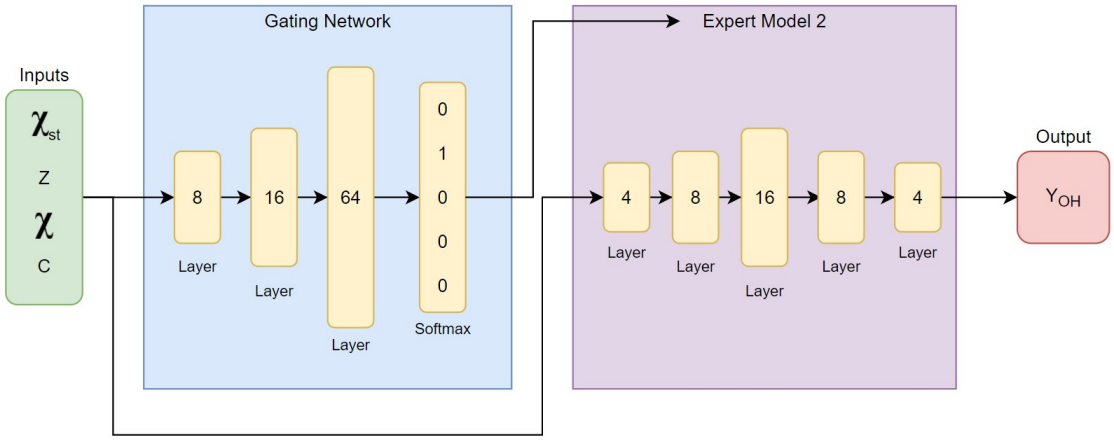

Figure 2.3: Detailed 5-cluster model structure flowchart.

The gating network is a DNN that is trained to perform classification based on the clusters identified by the clustering algorithms described above. The gating model has 3 hidden layers, progressively increasing in size from 8 to 16 to 64 before finally reaching a Softmax layer as shown in **Figure 2.3**. The Softmax layer assigns a decimal probability to each cluster describing the probability that the input belongs to a particular cluster. Using the gating network, the expert model with the highest probability is chosen and allowed to make a prediction.

The gating network and expert models used in this MoE framework were constructed using Keras. All training and testing was completed within Google Colaboratory, which serves as a Jupyter notebook executed on Google's cloud servers.

The expert models are complex DNNs that have been trained on a specific cluster as identified by the clustering algorithm. A DNN with 5 hidden layers is used, increasing in size from 4 to 16 nodes and then decreasing back in size to 4 nodes before the output layer which makes the final value prediction as shown in **Figure 2.3**. The DNNs were each trained for 300 epochs using the Adam optimizer [28] with an initial learning rate of 0.01. The model uses an adaptive learning rate-based system, which primarily serves to ensure that the model does not reach a plateau during the training process. This adaptive learning rate works by comparing the error in the model's prediction within a pre-defined number of epochs to identify whether the model has reached a

plateau. If a plateau is identified, the learning rate is decreased by a predefined factor, which was 0.4 for this research. This complex model architecture coupled with the adaptive learning rate significantly improved the model's performance as compared to previous approaches.

3. RESULTS

3.1 Clustering

Clustering of the input space was completed using a variety of algorithms. For each of these clustering algorithms, the number of clusters was defined before clustering the data. An example of the unsupervised learning-based clustering algorithm can be seen in **Figures 3.1-3.2** below using the Gaussian Mixture Model with 4 clusters.

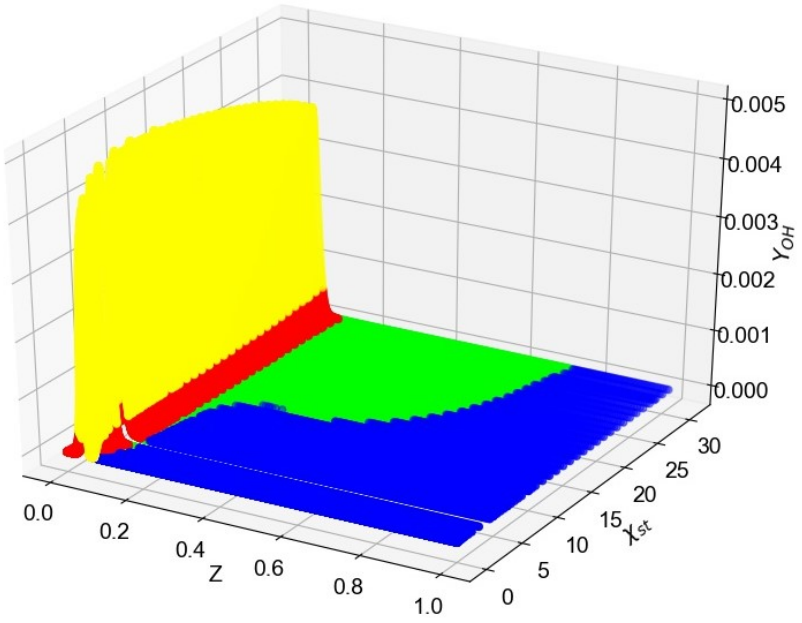

Figure 3.1: Clustered data using Gaussian Mixture Model with each color representing a different cluster.

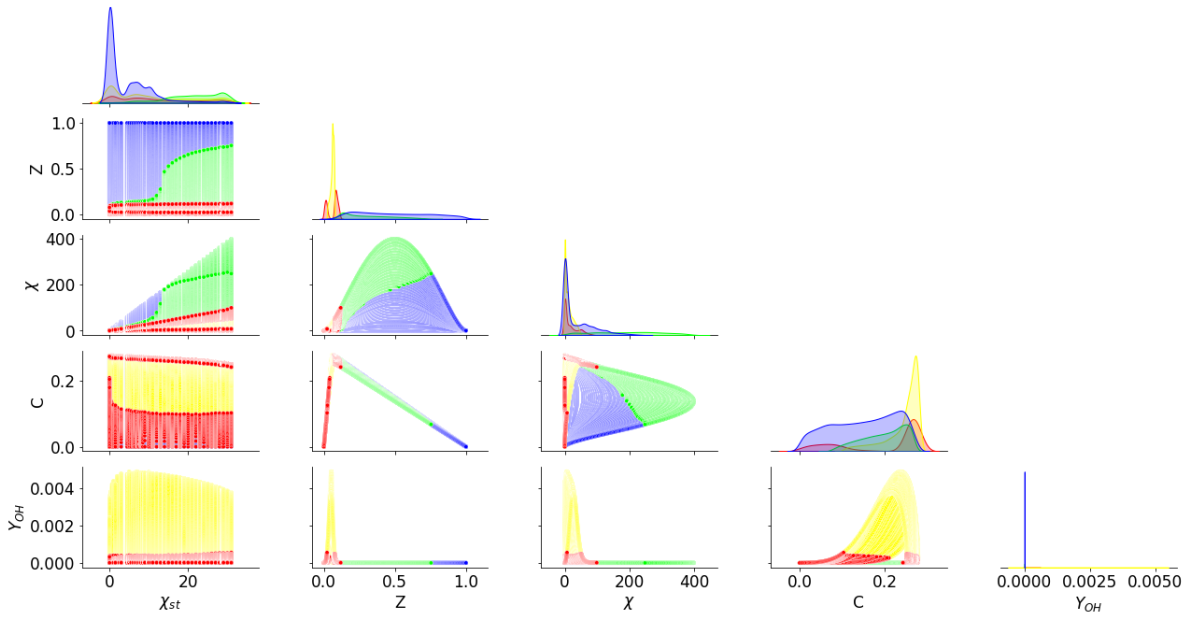

Figure 3.2: Detailed pairwise-plot of clustered data using Gaussian Mixture Model with each color representing a different cluster.

Figures 3.1-3.2 above provide a visualization of how the Gaussian Mixture Model algorithm clusters the input space with 4 clusters, with each color representing a different cluster. **Figure 3.1** shows the mass fraction of OH plotted against the two most important inputs, Z and χ_{st}. There is a clear and physical meaning to how the clusters are divided, as the boundaries between the various clusters are easily identifiable. The clusters identify the dataspaces that are identical and classify them as one cluster. This type of clustering ensures that even if the data is similar to each other with majority variables close to each other, the clustering will put them in different clusters depending on slight changes in important variables such as Z, λ, χ that govern the quenching and re-ignition regimes. **Figures 3.2** provides insight into the relationships between the various relevant variables. The diagonal plots show the density of each variable with respect to each cluster. It is clear that the blue cluster mainly consists of values at lower χ_{st} values and Y_{OH} values near 0. The yellow cluster, however, is primarily in a very specific Z range and higher values of Y_{OH}. This cluster contains the dataspace that corresponds to igniting flamelets.

3.2 Model Evaluation

Once the data had been clustered and the expert models trained, the complete MoE model structure was assembled and evaluated on new data that the models had not been trained on. The results of this evaluation are shown below in **Figures 3.3-3.4**.

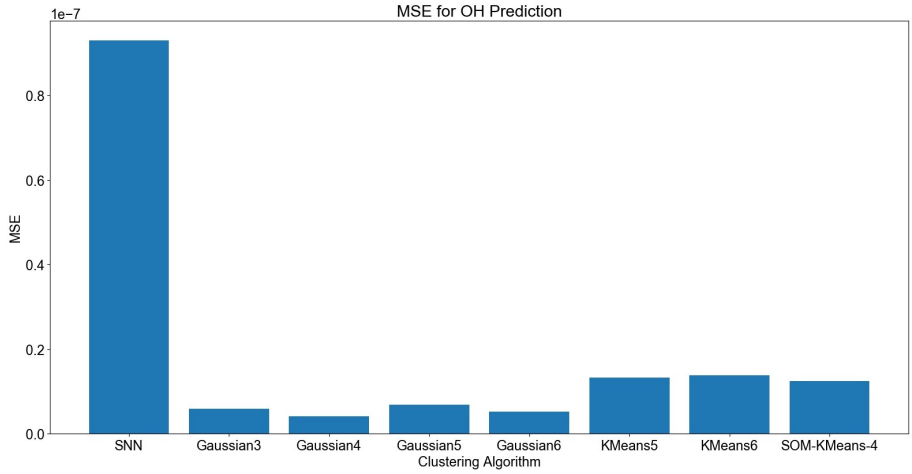

Figure 3.3: Mean squared error of evaluated clustering algorithms.

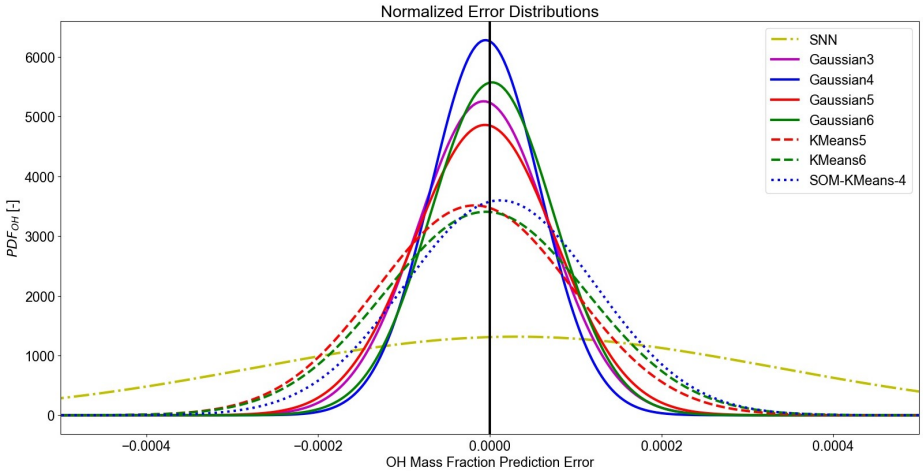

Figure 3.4: Normal distribution of evaluated clustering algorithms.

Figure 3.3 compares the prediction mean squared error (MSE) of several clustering algorithms with varied number of clusters. It can clearly be seen that the Gaussian Mixture Model provides a better clustering of the data, as they display the lowest error out of the models evaluated. It is clear that the SNN performs the worst as it has the highest error. This reinforces the notion that dividing the input space and training expert models is more accurate.

However, a clear trend is not observed in terms of increasing the number of clusters. This can be attributed to several factors. As the number of clusters increases, the training dataset of each cluster consequently decreases, meaning the DNN will have less data to learn from. Additionally, an increase in number of clusters results in a multiplying effect as the algorithm must choose from more clusters, which ultimately leads to a lower gating network accuracy.

Figure 3.4 displays normalized error distributions for each of the evaluated clustering algorithms. An ideal model would have a mean prediction error of 0 and an extremely tight distribution about its mean. The Gaussian Mixture Model with 4 clusters clearly performs the best out of the evaluated algorithms as it is closest to a mean prediction error of 0 in addition to having a tighter distribution around its mean prediction error. Therefore, the Gaussian Mixture Model with 4 clusters is the most accurate and precise clustering algorithm evaluated.

4. CONCLUSION

In this thesis, a new neural network architecture with an advanced learning rate system and an unsupervised learning-based gating network to predict the flamelet thermo-chemical scalars was presented. The following can be summarized from the results:

1. The gating network must be trained based on the results of an unsupervised clustering technique so as to identify the variability of inter-dependence between the multi-dimensional inputs.

2. There exists an optimum number of clusters. This is due to the fact that the accuracy of the architecture increases with increasing number of clusters only until a specific point. This point is defined by the accuracy of the gating network. Once reaching this point the gating network accuracy overcomes the advantages of diving the manifold further into clusters.

3. The choice of unsupervised clustering can be based on the pairwise-plot which reveals how one variable depends on other and how it is classified in a specific cluster. The idea is to have most clusters in the manifold with maximum variability to track any instances of quenching and re-ignition accurately.

4. The architecture proposed in this study works best with the Gaussian Mixture Model (4 clusters) unsupervised clustering based gating network to predict the OH mass fraction.

REFERENCES

[1] C. Rutland, "Large-eddy simulations for internal combustion engines–a review," *International Journal of Engine Research*, vol. 12, no. 5, pp. 421–451, 2011.

[2] T. Lu and C. K. Law, "Linear time reduction of large kinetic mechanisms with directed relation graph: n-heptane and iso-octane," *Combustion and flame*, vol. 144, no. 1-2, pp. 24–36, 2006.

[3] P. Pepiot-Desjardins and H. Pitsch, "An efficient error-propagation-based reduction method for large chemical kinetic mechanisms," *Combustion and Flame*, vol. 154, no. 1-2, pp. 67–81, 2008.

[4] L. Liang, J. G. Stevens, and J. T. Farrell, "A dynamic adaptive chemistry scheme for reactive flow computations," *Proceedings of the Combustion Institute*, vol. 32, no. 1, pp. 527–534, 2009.

[5] W. Sun, Z. Chen, X. Gou, and Y. Ju, "A path flux analysis method for the reduction of detailed chemical kinetic mechanisms," *Combustion and Flame*, vol. 157, no. 7, pp. 1298–1307, 2010.

[6] X. Gao, S. Yang, and W. Sun, "A global pathway selection algorithm for the reduction of detailed chemical kinetic mechanisms," *Combustion and Flame*, vol. 167, pp. 238–247, 2016.

[7] F. Contino, H. Jeanmart, T. Lucchini, and G. D'Errico, "Coupling of in situ adaptive tabulation and dynamic adaptive chemistry: An effective method for solving combustion in engine simulations," *Proceedings of the Combustion Institute*, vol. 33, no. 2, pp. 3057–3064, 2011.

[8] S. B. Pope, "Computationally efficient implementation of combustion chemistry using in situ adaptive tabulation," 1997.

[9] N. Peters, "Turbulent combustion," 2001.

[10] R. Barlow, J. Frank, A. Karpetis, and J.-Y. Chen, "Piloted methane/air jet flames: Transport effects and aspects of scalar structure," *Combustion and flame*, vol. 143, no. 4, pp. 433–449, 2005.

[11] O. Desjardins, G. Blanquart, G. Balarac, and H. Pitsch, "High order conservative finite difference scheme for variable density low mach number turbulent flows," *Journal of Computational Physics*, vol. 227, no. 15, pp. 7125–7159, 2008.

[12] N. Peters, "Laminar diffusion flamelet models in non-premixed turbulent combustion," *Progress in energy and combustion science*, vol. 10, no. 3, pp. 319–339, 1984.

[13] C. D PIERCE and P. Moin, "Progress-variable approach for large-eddy simulation of non-premixed turbulent combustion," *Journal of fluid Mechanics*, vol. 504, p. 73, 2004.

[14] M. Ihme, C. M. Cha, and H. Pitsch, "Prediction of local extinction and re-ignition effects in non-premixed turbulent combustion using a flamelet/progress variable approach," *Proceedings of the Combustion Institute*, vol. 30, no. 1, pp. 793–800, 2005.

[15] J. Van Oijen and L. De Goey, "Modelling of premixed laminar flames using flamelet-generated manifolds," *Combustion Science and Technology*, vol. 161, no. 1, pp. 113–137, 2000.

[16] H. Pitsch, M. Chen, and N. Peters, "Unsteady flamelet modeling of turbulent hydrogen-air diffusion flames," in *Symposium (international) on combustion*, vol. 27, pp. 1057–1064, Elsevier, 1998.

[17] M. Ihme and Y. C. See, "Prediction of autoignition in a lifted methane/air flame using an unsteady flamelet/progress variable model," *Combustion and Flame*, vol. 157, no. 10, pp. 1850–1862, 2010.

[18] C. Bajaj, M. Ameen, and J. Abraham, "Evaluation of an unsteady flamelet progress variable model for autoignition and flame lift-off in diesel jets," *Combustion Science and Technology*, vol. 185, no. 3, pp. 454–472, 2013.

[19] M. Ihme, C. Schmitt, and H. Pitsch, "Optimal artificial neural networks and tabulation methods for chemistry representation in les of a bluff-body swirl-stabilized flame," *Proceedings of the Combustion Institute*, vol. 32, no. 1, pp. 1527–1535, 2009.

[20] M. Emami and A. E. Fard, "Laminar flamelet modeling of a turbulent ch4/h2/n2 jet diffusion flame using artificial neural networks," *Applied Mathematical Modelling*, vol. 36, no. 5, pp. 2082–2093, 2012.

[21] O. Owoyele, P. Kundu, M. M. Ameen, T. Echekki, and S. Som, "Application of deep artificial neural networks to multi-dimensional flamelet libraries and spray flames," *International Journal of Engine Research*, vol. 21, no. 1, pp. 151–168, 2020.

[22] R. Ranade, G. Li, S. Li, and T. Echekki, "An efficient machine-learning approach for pdf tabulation in turbulent combustion closure," *Combustion Science and Technology*, pp. 1–20, 2019.

[23] O. Owoyele, P. Kundu, and P. Pal, "Efficient bifurcation and tabulation of multi-dimensional combustion manifolds using deep mixture of experts: An a priori study," *Proceedings of the Combustion Institute*, 2020.

[24] G. D'Alessio, A. Parente, A. Stagni, and A. Cuoci, "Adaptive chemistry via pre-partitioning of composition space and mechanism reduction," *Combustion and Flame*, vol. 211, pp. 68–82, 2020.

[25] H. Pitsch, "Flamemaster: A c++ computer program for 0d combustion and 1d laminar flame calculations," *Cited in*, vol. 81, 1998.

[26] G. P. Smith, "Gri-mech 3.0," *http://www. me. berkley. edu/gri_mech/*, 1999.

[27] F. Pedregosa, G. Varoquaux, A. Gramfort, V. Michel, B. Thirion, O. Grisel, M. Blondel, P. Prettenhofer, R. Weiss, V. Dubourg, J. Vanderplas, A. Passos, D. Cournapeau, M. Brucher, M. Perrot, and E. Duchesnay, "Scikit-learn: Machine learning in Python," *Journal of Machine Learning Research*, vol. 12, pp. 2825–2830, 2011.

[28] D. P. Kingma and J. Ba, "Adam: A method for stochastic optimization," *arXiv preprint arXiv:1412.6980*, 2014.