



IDDES modeling of a dual-mode scramjet by dynamic zone flamelet model with sensitivity analysis of zoning parameter

Zheng Zhang¹, Wei Yao²

Extended Abstract

The scramjet has attracted huge interest in recent decades because of the characteristics of much higher specific impulse and simple structure, which shows great potential in applications of fast long-range aircraft around the globe and the carrier vehicle for space exploration [1]. Due to the technical difficulties and massive cost in flight tests and the limitations of time and geometry scales in ground experiments, the computational fluid dynamics (CFD) method is necessary in fundamental studies or concept design for scramjet engines [2].

In the supersonic combustor, the strong shock waves have strong interactions with other flow patterns, such as boundary layers, shear layers and eddies. These processes couple with chemical reactions, result in the complex compressible turbulent combustion interaction (TCI) which rapidly temporal and spatial evolution within the combustion chamber [3]. Consequently, the flame in scramjet engines is intrinsically instable and contains a broad range of characteristic time and length scales, posing significant challenges in high fidelity turbulent and combustion modeling. Furthermore, in order to accurately capture various limiting combustion behaviours in the engine, such as extinction and re-ignition, flame mode transitions, etc., detailed kinetics with hundreds of species and reactions are required. Because of that, the large eddy simulation (LES) with detailed reaction mechanisms has become an inevitable trend in numerical studies of scramjet engines [4-6]. However, the high-resolution LES with the grid size of tens of millions or even billions needs a large amount of computational time and cost, especially for combustion modeling involving dozens or even hundreds of elementary reactions, which is computationally unaffordable for practical engineering applications.

To alleviate the massive computational cost, an attractive and effective way is to accelerate the solving of combustion chemistry, considering that over 50% of the CPU times is consumed in chemistry solving. There are two main technical routes targeting for that. One is the direct acceleration methods, which focus on mechanism reducing, such as DAC [7] and ISAT[8]. The another is manifold dimension reduction of thermochemistry states, which mapping the reactive scalars in the state-space constructed with conserved scalars, such as the flamelet based [9, 10] and conditional moment closure (CMC) methods [11, 12]. The manifold reduction model achieves a low dimensional solution for turbulent combustion, eliminating the need for time-consuming chemical reaction calculations at each cell of computational grid, as required in finite-rate models like PaSR and EDC.

Compared to subsonic combustion, high-speed supersonic combustion is characterized by high Reynolds number flow, where the time scales of chemical reactions and turbulent fluctuations are comparable, and small-scale turbulent eddies interact with the reaction zone of the flamelet. Therefore, the adaptability of flamelet-based models is challenged in high-speed supersonic turbulent combustion. On the other hand, CMC-type models are constructed based on the statistical concept of conditional

¹ State Key Laboratory of High Temperature Gas Dynamics, Institute of Mechanics, CAS, No. 15 Beisihuanxi Road, Beijing 100190, China, zhangzheng@imech.ac.cn

² State Key Laboratory of High Temperature Gas Dynamics, Institute of Mechanics, CAS, No. 15 Beisihuanxi Road, Beijing 100190, China, weiyao@imech.ac.cn

averaging, mapping flamelet (conditional moments) into the conditioning scalar space, without the physical assumption of thin flamelet and thus have broader applicability.

In the conventional CMC model, the transportation of conditioned scalar is resolved based on a static coarse grid divided by geometric coordinates. To accurately close the reaction terms in CMC model with a simple single-conditioned first order closure, it is necessary to satisfy a relative small fluctuation of the reactive species around their conditional mean in the CMC grid. However, for complex ignition and extinction phenomena presented in scramjet engines, the doubly conditioned moment methods or the second-order closure CMC model is required to accurately capture the significant fluctuations relative to the conditional mean. Although the doubly-conditioned and second-order moment methods improve the accuracy, the computational cost and model complexity are significantly increased [13, 14], making it less suitable for engineering applications. In recent years, based on the dynamic zoning concept, Yao [15, 16] proposed the Dynamic Zone Flamelet Model (DZFM), in which the cell of computational grid is clustered based on reacting related parameters (zoning parameters), such as mixture fraction, coordinates, and Mach number, to form the dynamic CMC grid (zone). The homogeneous chemistry state can be realized through clustering the computational grids based on appropriate zoning parameters, thus the fluctuations of species within each CMC zone are reduced. Because of that, a strong correlation between conditioning scalar (mixture fraction) and species is achieved, which can markedly improve the accuracy of single-conditioned first order moment closure in theory.

However, select an appropriate zoning parameters to satisfy accuracy required with CMC zones as few as possible is not an easy task. In previous study [15, 17], the zoning configuration is constructed relying on experience and prior knowledge about the physics among combustors. In this work, the sensitivity analysis of zoning parameters is conducted based on active subspace (AS) method [18]. The active subspace is defined by a set of important directions in the space composed of reaction related scalar. The dataspace for training the subspace is gathered from a PaSR modeling base on a model combustor. The major scalars in the active subspace having higher sensitivity to the chemical state, are selected as the zoning parameters. Finally, the DZFM model with a priori zoning configuration is employed to investigate the mode transition in a cavity based dual-mode scramjet combustor [19]. The combustor consists of a sonic hydrogen jet injected into a supersonic crossflow upstream of a wall cavity, the combustion mode transition is realized through increasing the stagnation temperatures (T_0) of the supersonic.

Firstly, the global sensitivity of the flame surface (Y_{OH}) to the related six parameters including mixture fraction mf , heat release rate dQ , reaction progress variable C_z , coordinates (x , y), and Mach number Ma , are evaluated by AS method. As shown in Fig.1 for the diffusion flame zone, mf is the most important variable of the one-dimensional active space \mathbf{w} . For the premixed flame zone, dQ and C_z contribute the most to the active space. Therefore, dQ and C_z are necessary zoning parameters to realize a homogeneous reaction state in each CMC zone for the premixed flame dominated combustor.

Both the cavity stabilized (CS) flame at $T_0 = 1050\text{ K}$ and the jet-wake stabilized (JWS) flame at $T_0 = 1370\text{ K}$ observed in the experiments are well reproduced as shown in Fig.2. According to the iso-surface of stoichiometry mixture fraction, it can be found that the JWS flame is a diffusion dominated flame while the CS is a premixed dominated flame. To validate the feasibility of AS method, two types of zoning configuration are utilized for the CS case. As shown in Fig.3, with similar size of CMC grids, the zoning configuration composed of dQ , C_z and mf well captured the cavity stabilized mode, the one with mf and X coordinate resulting a jet wake stabilized mode. A computational efficiency comparison between different zoning configuration will be conducted. Besides, the dynamic behaviors of flame and flow will be analyzed to reveal the mechanisms for flame mode transition.

Keywords: *Supersonic combustion, Dynamic zone flamelet model, IDDES, Zoning parameter, Sensitivity analysis*

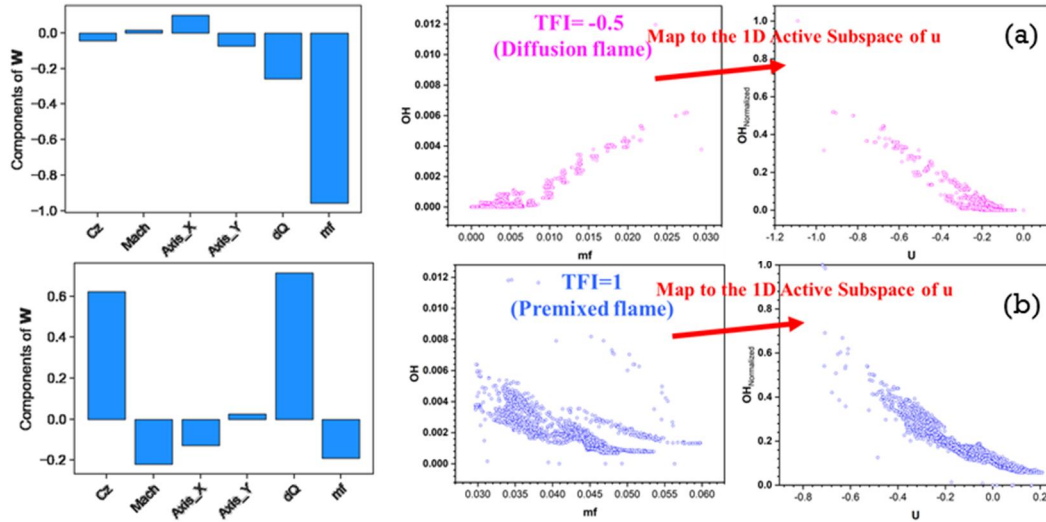


Fig 1. Sensitivity analysis for (a) the diffusion flame dominated zone with $TFI=-0.5$, and (b) the premixed flame dominated zone with $TFI=1$

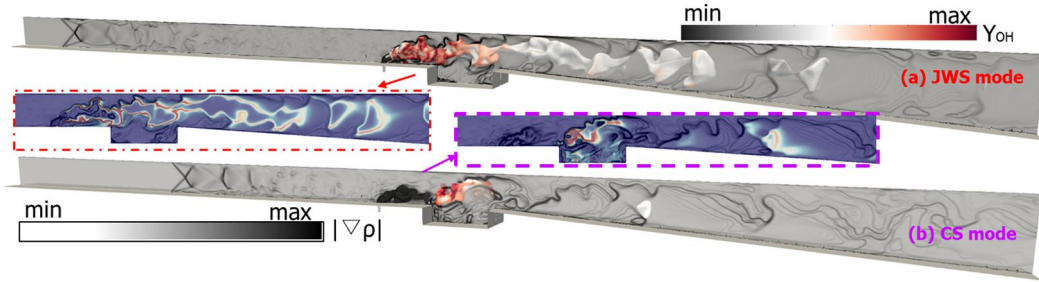


Fig 2. Numerical schlieren overlaid with Iso-surface of stoichiometry mixture fraction ($mf = 0.0295$) coloured by Y_{OH} for (a) jet-wake stabilized and (b) cavity stabilized cases.

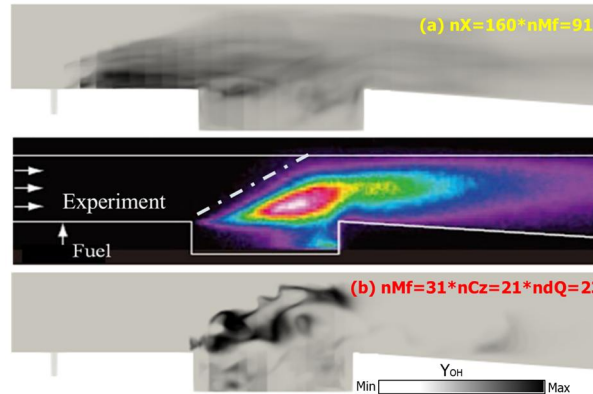


Fig 3. Comparison of spanwise superposition result of Y_{OH} with OH^* luminosity image from experiment [19] for different zoning configurations.

References

1. Urzay, J., "Supersonic Combustion in Air-Breathing Propulsion Systems for Hypersonic Flight," Vol. 50, No. 1, 2018, pp. 593-627. doi: 10.1146/annurev-fluid-122316-045217
2. Liu, Q., Baccarella, D., and Lee, T., "Review of Combustion Stabilization for Hypersonic Airbreathing Propulsion," *Progress in Aerospace Sciences*, Vol. 119, 2020, p. 100636. doi: <https://doi.org/10.1016/j.paerosci.2020.100636>

3. Wang, Z.-g., Sun, M.-b., Wang, H.-b., Yu, J.-f., Liang, J.-h., and Zhuang, F.-c., "Mixing-Related Low Frequency Oscillation of Combustion in an Ethylene-Fueled Supersonic Combustor," *Proceedings of the Combustion Institute*, Vol. 35, No. 2, 2015, pp. 2137-2144. doi: <https://doi.org/10.1016/j.proci.2014.09.005>
4. Nielsen, T. B., Edwards, J. R., Chelliah, H. K., Lieber, D., Geipel, C., Goynes, C. P., Rockwell, R. D., and Cutler, A. D., "Hybrid Large Eddy Simulation/Reynolds-Averaged Navier–Stokes Analysis of a Premixed Ethylene-Fueled Dual-Mode Scramjet Combustor," *AIAA Journal*, Vol. 59, No. 7, 2021, pp. 2440-2456. doi: 10.2514/1.J059343
5. Zhang, H., Zhao, M., and Huang, Z., "Large Eddy Simulation of Turbulent Supersonic Hydrogen Flames with Openfoam," *Fuel*, Vol. 282, 2020, p. 118812. doi: <https://doi.org/10.1016/j.fuel.2020.118812>
6. Fureby, C., "Subgrid Models, Reaction Mechanisms, and Combustion Models in Large-Eddy Simulation of Supersonic Combustion," *Aiaa Journal*, Vol. 59, No. 1, 2021, pp. 215-227. doi: 10.2514/1.J059597
7. Lu, T., and Law, C. K., "Toward Accommodating Realistic Fuel Chemistry in Large-Scale Computations," *Progress in Energy and Combustion Science*, Vol. 35, No. 2, 2009, pp. 192-215. doi: <https://doi.org/10.1016/j.peccs.2008.10.002>
8. Contino, F., Jeanmart, H., Lucchini, T., and D'Errico, G., "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, 2011, pp. 3057-3064. doi: <https://doi.org/10.1016/j.proci.2010.08.002>
9. Fan, Z., Liu, W., Sun, M., Wang, Z., Zhuang, F., and Luo, W., "Theoretical Analysis of Flamelet Model for Supersonic Turbulent Combustion," *Science China Technological Sciences*, Vol. 55, No. 1, 2012, pp. 193-205. doi: 10.1007/s11431-011-4659-7
10. Yamamoto, H., Toyonaga, R., Komatsu, Y., Kabayama, K., Mizobuchi, Y., and Sato, T., "Improved Methods of Laminar Flamelet Model for Compressible Flow," *AIAA Journal*, Vol. 58, No. 8, 2020, pp. 3514-3526. doi: 10.2514/1.J058247
11. Klimenko, A. Y., and Bilger, R. W., "Conditional Moment Closure for Turbulent Combustion," *Progress in Energy and Combustion Science*, Vol. 25, No. 6, 1999, pp. 595-687. doi: [https://doi.org/10.1016/S0360-1285\(99\)00006-4](https://doi.org/10.1016/S0360-1285(99)00006-4)
12. Han, K., and Huh, K. Y., "Conditional Moment Closure Method with Tabulated Chemistry in Adiabatic Turbulent Nonpremixed Jet Flames," *Combustion and Flame*, Vol. 234, 2021, p. 111652. doi: <https://doi.org/10.1016/j.combustflame.2021.111652>
13. Richardson, E. S., Yoo, C. S., and Chen, J. H., "Analysis of Second-Order Conditional Moment Closure Applied to an Autoignitive Lifted Hydrogen Jet Flame," *Proceedings of the Combustion Institute*, Vol. 32, No. 2, 2009, pp. 1695-1703. doi: <https://doi.org/10.1016/j.proci.2008.05.041>
14. Han, K., and Huh, K. Y., "First and Second Order Lagrangian Conditional Moment Closure Method in Turbulent Nonpremixed Flames," *Proceedings of the Combustion Institute*, Vol. 35, No. 2, 2015, pp. 1175-1182. doi: <https://doi.org/10.1016/j.proci.2014.07.058>
15. Yao, W., "On the Application of Dynamic Zone Flamelet Model to Large Eddy Simulation of Supersonic Hydrogen Flame," *International Journal of Hydrogen Energy*, Vol. 45, No. 41, 2020, pp. 21940-21955. doi: <https://doi.org/10.1016/j.ijhydene.2020.05.189>
16. Yao, W., and Fan, X., "Development of Zone Flamelet Model for Scramjet Combustor Modeling." 2017. doi: 10.2514/6.2017-2277
17. Zhang, Z., Yao, W., Wang, Q., and Zhao, W., "Iddes Simulation of Hydrogen-Fueled Supersonic Combustion Based on Dynamic Zone Flamelet Model," *Fuel*, Vol. 347, 2023. doi: 10.1016/j.fuel.2023.128502
18. Constantine, P. G., Emory, M., Larsson, J., and Iaccarino, G., "Exploiting Active Subspaces to Quantify Uncertainty in the Numerical Simulation of the Hyshot II Scramjet," *Journal of Computational Physics*, Vol. 302, 2015, pp. 1-20. doi: <https://doi.org/10.1016/j.jcp.2015.09.001>
19. Micka, D. J., and Driscoll, J. F., "Combustion Characteristics of a Dual-Mode Scramjet Combustor with Cavity Flameholder," *Proceedings of the Combustion Institute*, Vol. 32, No. 2, 2009, pp. 2397-2404. doi: <https://doi.org/10.1016/j.proci.2008.06.192>