

UDC 66.021.2.3.048

https://doi.org/10.33619/2414-2948/91/45

SIMPLIFICATION AND VERIFICATION OF O-XYLENE FUEL MECHANISM

©*Hou Ruida*, ORCID: 0009-0000-6126-0269, Jiangsu University of Science and Technology, Zhenjiang, China, 553774347@qq.com

УПРОЩЕНИЕ И ПРОВЕРКА ОРТОКСИЛОЛЬНОГО ТОПЛИВНОГО МЕХАНИЗМА

©*Хоу Жуйда*, ORCID: 0009-0000-6126-0269, Цзянсуский университет науки и технологии, г. Чжэньцзян, Китай, 553774347@qq.com

Abstract. The increasing demand for energy due to economic globalization has led to the exploration of different types of fuels, including aromatic hydrocarbon fuels. Xylene is an essential aromatic hydrocarbon fuel and an important component of kerosene. This study employs the error propagation directed relationship diagram (DRGEP) and sensitivity analysis (SA) to simplify the reaction mechanism of o-xylene. The ignition delay time and laminar flame velocity predicted by the fuel mechanism under different working conditions are compared with pre-simplified experimental data. The study proposes a mechanism consisting of 298 reactions and 64 components to describe the combustion reaction of xylene. The simplified mechanism's ability to reproduce experimental results is assessed, and the results reveal that the simplified mechanism effectively reproduces the experimental results, indicating its potential usefulness in practical applications. This study has significant implications for the development of more efficient and sustainable energy sources. By providing insights into the combustion behavior of xylene, researchers can develop more accurate models for predicting the performance of this fuel under a range of conditions. This, in turn, can inform the development of new technologies that can help meet the growing demand for energy in a more sustainable and environmentally friendly way. Overall, this study contributes to our understanding of the combustion behavior of xylene, highlighting its potential as a sustainable energy source and offering a potential avenue for further research in this field.

Аннотация. Растущий спрос на энергию в связи с экономической глобализацией привел к исследованию различных видов топлива, в том числе ароматических углеводородных топлив. Ксилол является одним из основных ароматических углеводородных топлив и важным компонентом керосина. В данном исследовании используется диаграмма направленных отношений распространения ошибок (DRGEP) и анализ чувствительности (SA) для упрощения механизма реакции о-ксилола. Время задержки воспламенения и скорость ламинарного пламени, предсказанные топливным механизмом при различных рабочих условиях, сравниваются с предварительно упрощенными экспериментальными данными. В исследовании предложен механизм, состоящий из 298 реакций и 64 компонентов, для описания реакции горения ксилола. Оценивается способно упрощенного механизма воспроизводить экспериментальные результаты, и результаты показывают, что упрощенный механизм эффективно воспроизводит экспериментальные результаты, что указывает на его потенциальную полезность в практических приложениях. Это исследование имеет значительные последствия для разработки более эффективных и устойчивых источников энергии. Получив представление о поведении ксилола при горении, исследователи могут разработать более точные модели для прогнозирования работы этого топлива в различных

условиях. В целом, данное исследование вносит вклад в наше понимание поведения ксилола при горении, подчеркивая его потенциал в качестве устойчивого источника энергии и предлагая потенциальный путь для дальнейших исследований в этой области.

Keywords: o-xylene, combustion chemistry, skeletal mechanism.

Ключевые слова: о-ксилол, химия горения, скелетный механизм.

Aromatic hydrocarbons are important components of commercial gasoline, diesel and jet fuel, and small aromatic compounds such as benzene, toluene and xylene are key components of gasoline. According to a recent survey (<http://pps.ms.northropgrumman.com/>), the average contains 25%, 33% and 16% aromatic hydrocarbons by volume, respectively. C₈H₁₀ aromatic hydrocarbons (xylene and ethylbenzene) make up a significant portion of the aromatic hydrocarbons found in commercial fuels. Xylene, which is found in crude oil, is a typical polysubstituted aromatic hydrocarbon. Known as C₈H₁₀, xylene is the product of replacing two hydrogens on the benzene ring with a methyl group. It consists of three isomers: o-xylene, m-xylene and p-xylene. Xylene is widely used in coating, resin, dye, ink and other industries to do solvent; Used in medicine, explosives, pesticides and other industries to do synthetic monomer or solvent; It can also be used as a high octane gasoline component, which is an important raw material of organic chemical industry. It can also be used to remove asphalt from car body. Hospital pathology department is mainly used for tissue and section transparency and dewaxing. They are an important component of commercial gasoline and are found in diesel fuel and kerosene. These compounds were also detected and identified as intermediates in the combustion of commercial fuels. However, due to limited kinetic data, the oxidation and pyrolysis processes of xylene are far from understood. Phase xylene is a very important aromatic hydrocarbon fuel. The combustion of hydrocarbon fuel is a very complicated chemical reaction process. The study of the reaction mechanism and process is beneficial to the control of the combustion reaction process.

At present, combustion performance prediction for internal combustion engines can be performed by real engine experiments or simulation. The former is costly, time consuming, and complicated to operate. Simulation, on the other hand, is fast, simple to operate, and accurate in its results, and has become an important tool for the design and optimization of various properties in internal combustion engines [1]. For the numerical simulation of combustion performance of internal combustion engines, the chemical reaction mechanism is an important prerequisite that enables it to be carried into smoothly. Although the detailed chemical reaction mechanism can reflect the details of the chemical reaction process more accurately and has great advantages in terms of realism and reliability, its size is too large and contains a large amount of chemical reaction kinetic information, which leads to a huge computational volume, and it is difficult to apply it directly to the three-dimensional numerical simulation of combustion. Therefore, a targeted simplification of the detailed chemical reaction mechanism is needed to reduce its components and primitive reactions and improve the computational efficiency of numerical simulations while ensuring the prediction accuracy [2].

In simulation, a detailed chemical reaction mechanism is required for computer calculation. Generally, detailed chemical reaction mechanism components and primitive reactions are many and complex, which take a lot of time to process in computer simulation, so a reasonable simplification and optimization of the mechanism can make the simulation consume less time while ensuring the accuracy of the results. The basic principle of mechanism simplification is to identify redundant

reactions and components, and then remove them from the detailed mechanism. The current methods of mechanism simplification are SA (Sensitivity analysis) [3], DRG (Directed relation graph) [4], and DRGEP (Directed relation graph with error propagation) [5], which is derived from the direct relation graph method. graph with error propagation) [5], DRGASA (DRG-aided sensitivity analysis), DRGEP SA (DRG with error propagation and sensitivity analysis), etc.

As far as I know, there are Battin-Leclerc et al [6] and Gaïl [8-10] and others who are mature in the study of the mechanism of xylenes, and Battin-Leclerc et al [6] are studying the three parts of the mechanism of xylenes separately, in which the mechanism for p-xylene is about 1200+ reactions and 180+ components, while Gaïl's [8-10] mechanism is more than 1000 reaction steps and more than 200 components. Experimental studies on the ignition delay time of paraxylene have only been reported by Battin-Leclerc et al [6] at an ignition pressure of 0.67-0.9 MPa and Shen et al [7] at an ignition pressure of 0.09-0.45 MPa, both of which were studied by the ignition conditions provided by the excitation tube, with the appearance of combustion reaction radicals as the ignition marker. Laminar flame velocities have experimental results from Han et al [11] at atmospheric pressures of 1 atm and 2 atm and an unburned gas body temperature of 353k.

CHEMKIN is a specialized software tool for solving complex chemical kinetic problems [12]. It is widely used in combustion, chemical reactions, microelectronics and automotive industries, as well as in atmospheric sciences. It was originally developed at Sandia National Laboratories and now acquired by the American company Reaction Design. CHEMKIN is very powerful and the software consists of three main core packages: gas-phase kinetics (GAS-Phase Kinetics), surface kinetics (Surface Kinetics) and transport properties (Transport Proces), on the basis of which more than 20 chemical reactor modules have been developed. Each reactor module has specific functions, and users can select different reactor modules to numerically simulate chemical reactions of complex systems. In addition, these modules can be used not only individually but also combined with other modules as needed to form a complex system. When using the software, the corresponding reaction mechanism should be imported as needed. For general combustion problems, if a zero-dimensional model is used, the mechanism file and thermodynamic data file should be imported; if a one-dimensional model is used, the mechanism file, thermodynamic data file and transport data file should be imported.

In this paper, the mechanism of Battin [6] et al. is selected as the detailed mechanism before simplification, and the detailed mechanism includes 1238 basic reactions involving 188 substances. This reaction mechanism well predicts the concentrations of reactants, products and intermediate species, the ignition delay time and the ignition process in the excitation tube, the ignition temperature of the back-diffusion flame, the species distribution in the jet premixed flame, and the propagation velocity of the laminar flow flame in the constant volume combustion chamber. Therefore, this mechanism is chosen as the detailed mechanism of xylene combustion reaction in this paper. Its ignition delay time was calculated using the fixed-volume adiabatic model in Chemkin software, and the premixed laminar flame model was used to calculate the laminar flame velocity and component concentration.

The non-essential species and basic reactions in the detailed mechanism are first removed by DRGEP. In this work, the components on the main path nodes are considered as target species. When the DRGEP threshold was set to 0.05 and the relative error of ignition delay time and laminar flame velocity was set to 20%, a skeleton mechanism consisting of 64 species and 375 elementary reactions was obtained.

Next, the above skeleton mechanism was further simplified using SA. The sensitivity coefficients of all primitive reactions were ranked and then filtered one by one from small to large.

The skeleton mechanism of xylenes with 330 primitive reactions for 64 components was constructed while ensuring that the ignition delay time and laminar flame speed were within the initial relative error.

The laminar flame velocity is an important indicator to judge the characteristics of the chemical reaction mechanism, and we compared the detailed mechanism and the simplified skeleton mechanism with the experimental results such as han [11]. The detailed mechanism and the simplified mechanism were compared in Figure 1 for the equivalent ratios of 0.7-1.5 and atmospheric pressures of 1 atm and 2 atm.

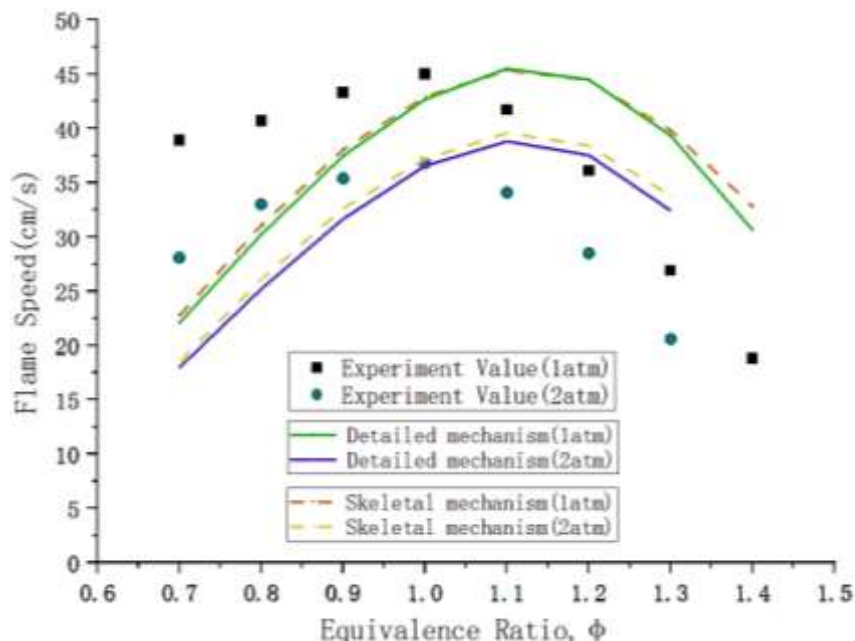


Figure 1. Comparison of laminar flame velocity of xylene predicted by the simplified before and after mechanism with experimental values

From Figure 1 we can see that the predicted value is lower than the experimental value in the poor ignition state, and conversely, the predicted value is higher than the experimental value in the rich ignition state, and the same mechanism trend before and after simplification is used to predict the laminar flame speed with less error.

Ignition delay time is also an important indicator to judge the effectiveness of the chemical reaction mechanism. During the ignition delay time, the fuel and oxidizer undergo some complex physical and chemical changes, which in turn affect the combustion pattern and emission characteristics of the internal combustion engine. We compare the detailed mechanism and the simplified skeleton mechanism with the experimental data of shen [7] et al. The results of the comparison are shown in Figure 2 for the operating conditions with equivalent ratios of 0.5 and 1.0, atmospheric pressures of 10 atm and 40 atm, and initial temperatures of 1000k-1300k, respectively.

From Figure 2, we can see that the predicted value of the mechanism is high, but the basic trend is the same. The simplified skeleton mechanism is high compared with the detailed mechanism, but the difference is small, so we can see that the simplified mechanism can be used to replace the detailed mechanism for prediction.

In this paper, a simplified mechanism for xylenes containing 330 radical reactions of 64 components was obtained by DRGEP, SA square. Under different conditions, the simplified mechanism was compared and analyzed with the experimental data and the detailed mechanism, and the ignition delay time and laminar flame velocity were similar to those predicted by the

original mechanism, and the simplified mechanism for xylenes could respond well to the ignition delay time and laminar flame velocity, and this simplified mechanism could be used to predict the combustion reaction of xylenes.

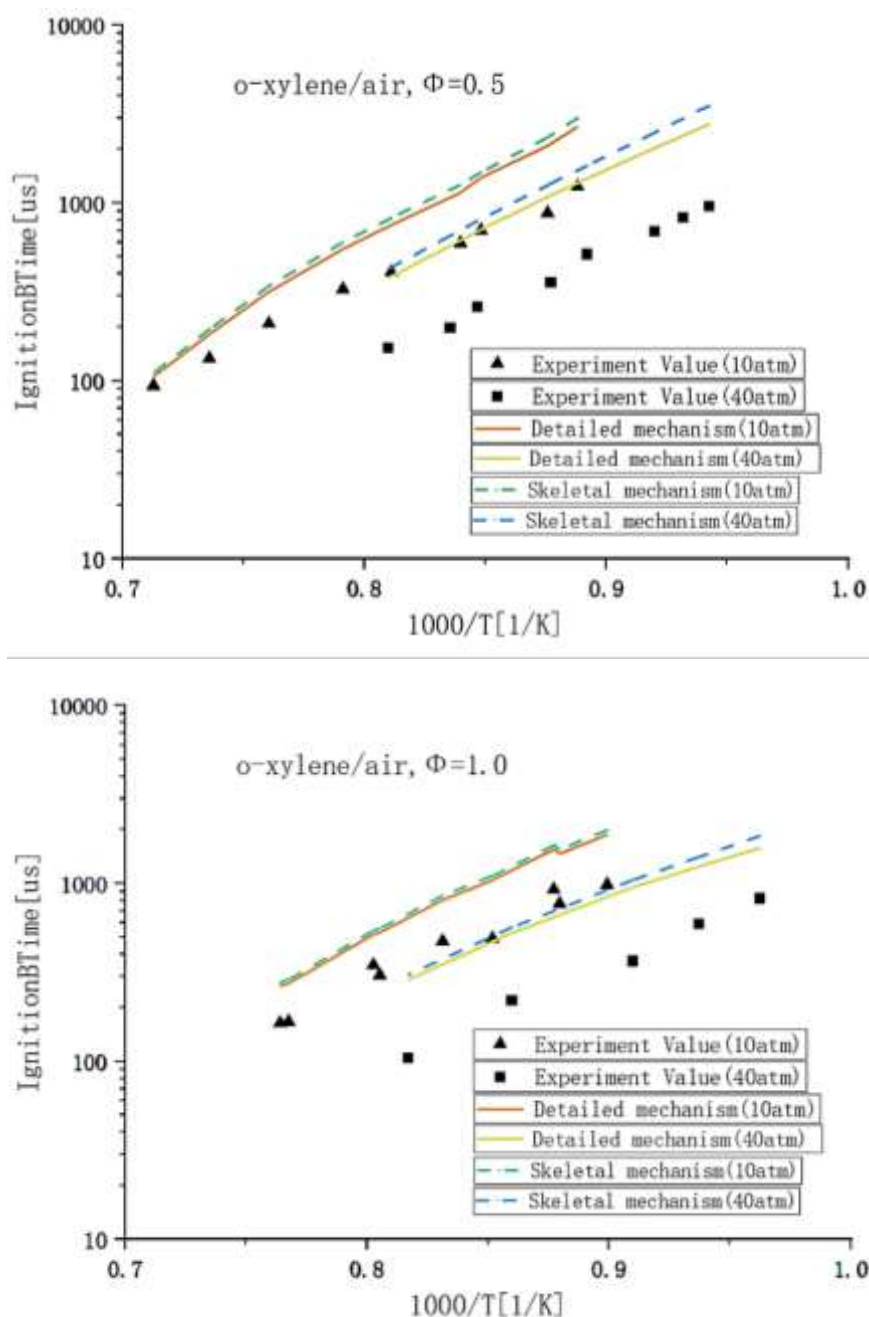


Figure 2. Comparison of the xylene ignition delay time predicted by the mechanism before and after simplification with the experimental value

References:

1. Tu, Y., Xu, S., Xu, M., Liu, H., & Yang, W. (2020). Numerical study of methane combustion under moderate or intense low-oxygen dilution regime at elevated pressure conditions up to 8 atm. *Energy*, 197, 117158. <https://doi.org/10.1016/j.energy.2020.117158>
2. Yang, M. (2021). Simplification of PODE_3/DME hybrid fuel mechanism and its effect on engine combustion process and emission generation. *Jiangsu University of Science and Technology*.

3. Turányi, T. (1990). Sensitivity analysis of complex kinetic systems. Tools and applications. *Journal of mathematical chemistry*, 5(3), 203-248. <https://doi.org/10.1007/BF01166355>
4. Lu, T., & Law, C. K. (2005). A directed relation graph method for mechanism reduction. *Proceedings of the Combustion Institute*, 30(1), 1333-1341. <https://doi.org/10.1016/j.proci.2004.08.145>
5. Pepiot-Desjardins, P., & Pitsch, H. (2008). An efficient error-propagation-based reduction method for large chemical kinetic mechanisms. *Combustion and Flame*, 154(1-2), 67-81. <https://doi.org/10.1016/j.combustflame.2007.10.020>
6. Battin-Leclerc, F., Bounaceur, R., Belmekki, N., & Glaude, P. A. (2006). Experimental and modeling study of the oxidation of xylenes. *International Journal of Chemical Kinetics*, 38(4), 284-302. <https://doi.org/10.1002/kin.20160>
7. Shen, H. P. S., & Oehlschlaeger, M. A. (2009). The autoignition of C₈H₁₀ aromatics at moderate temperatures and elevated pressures. *Combustion and Flame*, 156(5), 1053-1062. <https://doi.org/10.1016/j.combustflame.2008.11.015>
8. Gail, S., & Dagaut, P. (2005). Experimental kinetic study of the oxidation of p-xylene in a JSR and comprehensive detailed chemical kinetic modeling. *Combustion and flame*, 141(3), 281-297. <https://doi.org/10.1016/j.combustflame.2004.12.020>
9. Gail, S., & Dagaut, P. (2007). Oxidation of m-xylene in a JSR: experimental study and detailed chemical kinetic modeling. *Combustion science and technology*, 179(5), 813-844.
10. Gail, S., Dagaut, P., Black, G., & Simmie, J. M. (2023). *Combust. Sci. Technol.*
11. Han, D., Deng, S., Liang, W., Zhao, P., Wu, F., Huang, Z., & Law, C. K. (2017). Laminar flame propagation and nonpremixed stagnation ignition of toluene and xylenes. *Proceedings of the Combustion Institute*, 36(1), 479-489. <https://doi.org/10.1016/j.proci.2016.05.013>
12. Meng, Z., Wang, J., Qi, J., Xiong, C., Hou, L., & Luo, J. (2020). A simplified and optimized chemical mechanism for combustion of n-pentane at atmospheric pressure. *Processes*, 8(8), 884. <https://doi.org/10.3390/pr8080884>

Список литературы:

1. Tu Y., Xu S., Xu M., Liu H., Yang W. Numerical study of methane combustion under moderate or intense low-oxygen dilution regime at elevated pressure conditions up to 8 atm // *Energy*. 2020. V. 197. P. 117158. <https://doi.org/10.1016/j.energy.2020.117158>
2. Yang M. Simplification of PODE₃/DME hybrid fuel mechanism and its effect on engine combustion process and emission generation // Jiangsu University of Science and Technology. 2021.
3. Turányi T. Sensitivity analysis of complex kinetic systems. Tools and applications // *Journal of mathematical chemistry*. 1990. V. 5. №3. P. 203-248. <https://doi.org/10.1007/BF01166355>
4. Lu T., Law C. K. A directed relation graph method for mechanism reduction // *Proceedings of the Combustion Institute*. 2005. V. 30. №1. P. 1333-1341. <https://doi.org/10.1016/j.proci.2004.08.145>
5. Pepiot-Desjardins P., Pitsch H. An efficient error-propagation-based reduction method for large chemical kinetic mechanisms // *Combustion and Flame*. 2008. V. 154. №1-2. P. 67-81. <https://doi.org/10.1016/j.combustflame.2007.10.020>
6. Battin-Leclerc F., Bounaceur R., Belmekki N., Glaude P. A. Experimental and modeling study of the oxidation of xylenes // *International Journal of Chemical Kinetics*. 2006. V. 38. №4. P. 284-302. <https://doi.org/10.1002/kin.20160>

7. Shen H. P. S., Oehlschlaeger M. A. The autoignition of C₈H₁₀ aromatics at moderate temperatures and elevated pressures // *Combustion and Flame*. 2009. V. 156. №5. P. 1053-1062. <https://doi.org/10.1016/j.combustflame.2008.11.015>

8. Gail S., Dagaut P. Experimental kinetic study of the oxidation of p-xylene in a JSR and comprehensive detailed chemical kinetic modeling // *Combustion and flame*. 2005. V. 141. №3. P. 281-297. <https://doi.org/10.1016/j.combustflame.2004.12.020>

9. Gail S., Dagaut P. Oxidation of m-xylene in a JSR: experimental study and detailed chemical kinetic modeling // *Combustion science and technology*. 2007. V. 179. №5. P. 813-844.

10. Gail S., Dagaut P., Black G., Simmie J. M. *Combust. Sci. Technol.* 2023.

11. Han D., Deng S., Liang W., Zhao P., Wu F., Huang Z., Law C. K. Laminar flame propagation and nonpremixed stagnation ignition of toluene and xylenes // *Proceedings of the Combustion Institute*. 2017. V. 36. №1. P. 479-489. <https://doi.org/10.1016/j.proci.2016.05.013>

12. Meng Z., Wang J., Qi J., Xiong C., Hou L., Luo J. A simplified and optimized chemical mechanism for combustion of n-pentane at atmospheric pressure // *Processes*. 2020. V. 8. №8. P. 884. <https://doi.org/10.3390/pr8080884>

*Работа поступила
в редакцию 11.05.2023 г.*

*Принята к публикации
18.05.2023 г.*

Ссылка для цитирования:

Hou Ruida Simplification and Verification of O-xylene Fuel Mechanism // *Бюллетень науки и практики*. 2023. Т. 9. №6. С. 381-387. <https://doi.org/10.33619/2414-2948/91/45>

Cite as (APA):

Hou, Ruida (2023). Simplification and Verification of O-xylene Fuel Mechanism. *Bulletin of Science and Practice*, 9(6), 381-387. <https://doi.org/10.33619/2414-2948/91/45>