

# ВОСПЛАМЕНЕНИЕ СТЕХИОМЕТРИЧЕСКОЙ СМЕСИ АЦЕТОНА С КИСЛОРОДОМ ЗА ОТРАЖЕННЫМИ УДАРНЫМИ ВОЛНАМИ: ЧИСЛЕННОЕ МОДЕЛИРОВАНИЕ КИНЕТИКИ СВЕЧЕНИЯ $\text{OH}^*$ И $\text{CO}_2^*$ И ПОГЛОЩЕНИЯ $\text{CO}_2$ <sup>§</sup>

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**Аннотация:** Проведено численное моделирование воспламенения стехиометрической смеси  $0,5\%(\text{CH}_3)_2\text{CO} + 2\%\text{O}_2$  в аргоне за отраженными ударными волнами в диапазоне температур 1310–1810 К при давлениях 1 и 5 атм. Для расчетов использовался ряд детальных кинетических механизмов (ДКМ), представленных в литературе. Сравнение расчетных значений задержек воспламенения проводилось с экспериментальными данными по свечению  $\text{OH}^*$ ,  $\text{CO}_2^*$  и поглощению  $\text{CO}_2$ . Установлено, что представленные в литературе различные ДКМ описывают наблюдаемые задержки воспламенения и профили эмиссии с различной степенью точности.

**Ключевые слова:** кинетика воспламенения; численное моделирование; детальный кинетический механизм; задержка воспламенения; электронно-возбужденные состояния радикалов

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## Литература

1. *Tsuboi T., Ishii K., Tamura S.* Thermal oxidation of acetone behind reflected shock wave // *Nihon Kikai Gakkai Ronbunshu, B Hen Part B Trans. Japan Soc. Mech. Eng.*, 2001. Vol. 67. P. 2797–2804.
2. *Pichon S., Black G., Chaumeix N., Yahyaoui M., Simmie J. M., Curran H. J., Donohue R.* The combustion chemistry of a fuel tracer: Measured flame speeds and ignition delays and a detailed chemical kinetic model for the oxidation of acetone // *Combust. Flame*, 2009. Vol. 156. P. 494–504.
3. *Akih-Kumgeh B., Berghorson J. M.* Ignition of C3 oxygenated hydrocarbons and chemical kinetic modeling of propanal oxidation // *Combust. Flame*, 2011. Vol. 158. No. 10. P. 1877–1889.
4. *Chong Ch. T., Hochgreb S.* Measurements of laminar flame speeds of acetone/methane/air mixtures // *Combust. Flame*, 2011. Vol. 158. No. 3. P. 490–500.
5. *Singh H. B., O'Hara D., Herlth D., Sachse W., Blake D. R., Bradshaw J. D., Kanakidou M., Crutzen P. J.* Acetone in the atmosphere: Distribution, sources, and sinks // *J. Geophys. Res. Atmos.*, 1994. Vol. 99. P. 1805–1819.
6. *Yujing M., Mellouki A.* The near-UV absorption cross sections for several ketones // *J. Photoch. Photobio. A*, 2000. Vol. 134(1-2). P. 31–36.
7. *Saxena S., Kiefer J. H., Klippenstein S. J.* A shock-tube and theory study of the dissociation of acetone and subsequent recombination of methyl radicals // *32rd Symposium (International) on Combustion Proceedings*. — Pittsburgh, PA, USA: The Combustion Institute, 2009. P. 123–130.
8. *Wang H., Warner S. J., Oehlschlaeger M. A., Bounaceur R., Biet J., Glaude P. A.* An experimental and kinetic modeling study of the autoignition of  $\alpha$ -methyl-naphthalene/air and  $\alpha$ -methyl-naphthalene/*n*-decane/air mixtures at elevated pressures // *Combust. Flame*, 2010. Vol. 157. P. 1976–1978.
9. *Metcalfe W. K., Burke S. M., Ahmed S. S., Curran H. J.* A hierarchical and comparative kinetic modeling study of C<sub>1</sub>–C<sub>2</sub> hydrocarbon and oxygenated fuels // *Int. J. Chem. Kinet.*, 2013. Vol. 45. P. 638–675.
10. *Battin-Leclerc F., Warth V., Bounaceur R., Glaude P.-A., Herbinet O.* The oxidation of large alkylbenzenes: An experimental and modeling study // *35th Symposium (International) on Combustion Proceedings*. — Pittsburgh, PA, USA: The Combustion Institute, 2014. P. 349–356.
11. *Smirnov V. N., Tereza A. M., Vlasov P. A., Zhiltsova I. V.* Luminescent characteristics of the shock-wave ignition of an ethylene–oxygen mixture // *Combust. Sci. Technol.*, 2017. Vol. 189. No. 5. P. 854–868.
12. *Hall J. M., de Vries J., Amadio A. R., Petersen E. L.* Towards a kinetics model of CH chemiluminescence. *AIAA Paper No. 2005-1318*, 2005.
13. *Bozkurt M., Fikri M., Schulz C.* Investigation of the kinetics of  $\text{OH}^*$  and  $\text{CH}^*$  chemiluminescence in hydrocarbon

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- oxidation behind reflected shock waves // *Appl. Phys. B*, 2012. Vol. 107. No. 3. P. 515–527.
14. *Aul C. J., Metcalfe W. K., Burke S. M., Curran H. J., Petersen E. L.* Ignition and kinetic modeling of methane and ethane fuel blends with oxygen: A design of experiments approach // *Combust. Flame*, 2013. Vol. 160. P. 1153–1167.
15. *Власов П. А., Демиденко Т. С., Смирнов В. Н., Тереза А. М., Аткин Э. В.* Хемилюминесцентное свечение  $\text{CH}^*$ ,  $\text{C}_2^*$ ,  $\text{OH}^*$ ,  $\text{CO}_2^*$  при воспламенении этана за отраженными ударными волнами // *Хим. физика*, 2016. Т. 35. № 11. P. 54–61. doi: 10.7868/S0207401X16110133.
16. *Гейдон А., Герл И.* Ударная труба в химической физике высоких температур / Пер. с англ. — М.: Мир. 1966. 427 с. (*Gaydon A. G., Hurle I. R.* The shock tube in high-temperature chemical physics. — Springer US, 1963. 367 p.)
17. *Tereza A. M., Smirnov V. N., Vlasov P. A., Shumova V. V., Garmash A. A.* Emission of  $\text{OH}^*$  and  $\text{CO}_2^*$  during the high-temperature oxidation of acetone in reflected shock waves // *J. Phys. Conf. Ser.*, 2017. Vol. 946. P. 012071.
18. *Kee R. J., Rupley F. M., Meeks E., Miller J. A.* CHEMKIN III: Technical Report No. SAND96-8216. Sandia National Laboratories, Livermore, CA, USA, 1996.
19. *Ranzi E., Frassoldati A., Grana R., Cuoci A., Faravelli T., Kelley A. P., Law C. K.* Hierarchical and comparative kinetic modeling of laminar flame speeds of hydrocarbon and oxygenated fuels // *Prog. Energ. Combust.*, 2012. Vol. 38(4). P. 468–501. doi: 10.1016/j.peccs.2012.03.004.

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# IGNITION OF A STOICHIOMETRIC ACETONE–OXYGEN MIXTURE BEHIND REFLECTED SHOCK WAVES: NUMERICAL SIMULATION OF THE KINETICS OF LUMINESCENCE OF OH\* AND CO<sub>2</sub>\* AND ABSORPTION OF CO<sub>2</sub>

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**Abstract:** A numerical simulation of the ignition of a 0.5%(CH<sub>3</sub>)<sub>2</sub>CO + 2%O<sub>2</sub> + Ar mixture behind reflected shock waves in the temperature range 1310–1810 K at pressures of 1 and 5 atm has been performed. A number of detailed kinetic mechanisms (DKMs) reported in the literature have been tested. The calculated values of the ignition delay time have been compared to the respective experimental data obtained by monitoring the emission of OH\* and CO<sub>2</sub>\* and the absorption of CO<sub>2</sub>. It was demonstrated that the different DKMs presented in the literature describe the measured ignition delay times and emission profiles with varying degrees of accuracy.

**Keywords:** kinetics of ignition; numerical simulations; detailed kinetic mechanism; ignition delay time; electronically excited states of radicals

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## References

1. Tsuboi, T., K. Ishii, and S. Tamura. 2001. Thermal oxidation of acetone behind reflected shock wave. *Nihon Kikai Gakkai Ronbunshu, B Hen Part B Trans. Japan Soc. Mech. Eng.* 67:2797–2804.
2. Pichon, S., G. Black, N. Chaumeix, M. Yahyaoui, J. M. Simmie, H. J. Curran, and R. Donohue. 2009. The combustion chemistry of a fuel tracer: Measured flame speeds and ignition delays and a detailed chemical kinetic model for the oxidation of acetone. *Combust. Flame* 156:494–504.
3. Akih-Kumgeh, B., and J. M. Bergthorson. 2011. Ignition of C<sub>3</sub> oxygenated hydrocarbons and chemical kinetic modeling of propanal oxidation. *Combust. Flame* 158(10):1877–1889.
4. Chong, Ch. T., and S. Hochgreb. 2011. Measurements of laminar flame speeds of acetone/methane/air mixtures. *Combust. Flame* 158(3):490–500.
5. Singh, H. B., D. O’Hara, D. Herlth, W. Sachse, D. R. Blake, J. D. Bradshaw, M. Kanakidou, and P. J. Crutzen. 1994. Acetone in the atmosphere: Distribution, sources, and sinks. *J. Geophys. Res. Atmos.* 99:1805–1819.
6. Yujing, M., and A. Mellouki. 2000. The near-UV absorption cross sections for several ketones. *J. Photoch. Photobio. A* 134(1-2):31–36.
7. Saxena, S., J. H. Kiefer, and S. J. Klippenstein. 2009. A shock-tube and theory study of the dissociation of acetone and subsequent recombination of methyl radicals. *32rd Symposium (International) on Combustion Proceedings*. Pittsburgh, PA: The Combustion Institute. 123–130.
8. Wang, H., S. J. Warner, M. A. Oehlschlaeger, R. Bounaceur, J. Biet, and P. A. Glaude. 2010. An experimental and kinetic modeling study of the autoignition of  $\alpha$ -methyl-naphthalene/air and  $\alpha$ -methyl-naphthalene/*n*-decane/air mixtures at elevated pressures. *Combust. Flame* 157:1976–1978.
9. Metcalfe, W. K., S. M. Burke, S. S. Ahmed, and H. J. Curran. 2013. A hierarchical and comparative kinetic modeling study of C<sub>1</sub>–C<sub>2</sub> hydrocarbon and oxygenated fuels. *Int. J. Chem. Kinet.* 45:638–675.
10. Battin-Leclerc, F., V. Warth, R. Bounaceur, P.-A. Glaude, and O. Herbinet. 2014. The oxidation of large alkylbenzenes: An experimental and modeling study. *35th Symposium (International) on Combustion Proceedings*. Pittsburgh, PA: The Combustion Institute. 349–356.

11. Smirnov, V. N., A. M. Tereza, P. A. Vlasov, and I. V. Zhiltsova. 2017. Luminescent characteristics of the shock-wave ignition of an ethylene–oxygen mixture. *Combust. Sci. Technol.* 189(5):854–868.
12. Hall, J. M., J. de Vries, A. R. Amadio, and E. L. Petersen. 2005. Towards a kinetics model of CH chemiluminescence. AIAA Paper No. 2005-1318.
13. Bozkurt, M., M. Fikri, and C. Schulz. 2012. Investigation of the kinetics of OH\* and CH\* chemiluminescence in hydrocarbon oxidation behind reflected shock waves. *Appl. Phys. B* 107(3):515–527.
14. Aul, C. J., W. K. Metcalfe, S. M. Burke, H. J. Curran, and E. L. Petersen. 2013. Ignition and kinetic modeling of methane and ethane fuel blends with oxygen: A design of experiments approach. *Combust. Flame* 160:1153–1167.
15. Vlasov, P. A., T. S. Demidenko, V. N. Smirnov, A. M. Tereza, and E. V. Atkin. 2016. Chemiluminescent emission of CH\*, C<sub>2</sub>\*, OH\*, and CO<sub>2</sub>\* during the ignition of ethane behind reflected shock waves. *Russ. J. Phys. Chem. B* 10(6):983–990.
16. Gaydon, A. G., and I. R. Hurlle. 1963. *The shock tube in high-temperature chemical physics*. Springer US. 367 p.
17. Tereza, A. M., V. N. Smirnov, P. A. Vlasov, V. V. Shumova, and A. A. Garmash. 2017. Emission of OH\* and CO<sub>2</sub>\* during the high-temperature oxidation of acetone in reflected shock waves. *J. Phys. Conf. Ser.* 946:012071.
18. Kee, R. J., F. M. Rupley, E. Meeks, and J. A. Miller. 1966. CHEMKIN III: Tech. Report No. SAND96-8216. Sandia National Laboratories, Livermore, CA.
19. Ranzi, E., A. Frassoldati, R. Grana, A. Cuoci, T. Faravelli, A. P. Kelley, and C. K. Law. 2012. Hierarchical and comparative kinetic modeling of laminar flame speeds of hydrocarbon and oxygenated fuels. *Prog. Energ. Combust.* 38(4):468–501. doi: 10.1016/j.pecc.2012.03.004.

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