Numerical Study of Hydrogen Peroxide Thermal Decomposition in a Shock Tube

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Hydrogen peroxide (H2O2) has its significance during the combustion of heavy hydrocarbons in the internal combustion (IC) engines. Owing to its importance the measurements of H2O2 dissociation rate have been reported mostly using the shock tube apparatus. These types of experimental measurements are although quite reliable but require high cost. On the other hand, numerical simulations provide low cost and reliable solutions especially using computation fluid dynamics (CFD) software. In the current study an experimental shock tube flow is modeled using open access platform OpenFOAM to investigate the thermal decomposition of H2O2. Using two different convective schemes, limitedLinear and upwind, the propagation of shock wave and resultant dissociation reaction are simulated. The results of the simulations are compared with the experimental data. It is observed that the rate constant measured using the simulation data deviates from the experimental results in the low temperature range and approaches the experimental values as the temperature is raised.

Keywords: Reaction kinetics, Rate constant, Numerical simulation, Shock wave, Reflected shock wave, Contact discontinuity, Expansion fan, Internal flow, Compressible flow, Gas dynamics

Introduction

During the combustion of fossil fuels in the internal combustion engines, numerous intermediate reactions occur before the production of final products (Bhaskaran et al. 2002). Hydrogen peroxide is one of the most important intermediate compounds formed which guides and controls the downstream chain of reactions in the temperature range of 850 K to 1200 K (Hong et al. 2011). Hydrogen peroxide is also used as monopropellant using the catalytic decomposition technique in some types of rocket engines. It has its future as a green monopropellant (Westbrook 2000). For the delivery of micro satellites in the orbits, it is an established monopropellant fuel (Davenas et al. 2004). It is also being utilized as an oxidizer in some rocket engines. It has also found its utility for the alignment of satellites and attitude control purposes. Besides hydrogen peroxide has numerous industrial applications; for instance treatment of waste water, industrial waste treatment, bleaching of textile products and bleaching of paper etc.

Due to its versatile applications, H2O2 dissociate reaction is extensively used experimentally. Most experimental setups used shock tube. In the shock tube environment, the propagating shock wave upon reflection from end wall provides appropriate environment (in terms of temperature and pressure) where the thermal decomposition can occur (Anderson 2003). This process has been studied using various diagnostic techniques. Bilwakesh et al. (1968) performed the thermal decompo-
sition analysis with the help of experimental shock tube facility. In order to monitor the thermal decomposition they utilized the absorption methods. The driver section consisted of air and helium mixture whereas the driven section consisted of H$_2$O$_2$ and nitrogen mixture. The nitrogen served as the bath gas. Meyer et al. (1969) analyzed the decomposition of N$_2$H$_4$ and H$_2$O$_2$. They measured the decomposition rate of H$_2$O$_2$ between temperatures 950 K to 1450 K and the pressure was kept up to 20 bar. UV absorption was used to monitor the decomposition rates.

Few other studies such as Trainor et al. (1974) conducted the study of reunification of OH ion using the photolysis technique at low pressure and temperature and utilized the absorption spectroscopy. Using flash photolysis Zellner et al. (1988) conducted experiments at low temperature and pressure range. Forster et al. (1995) with the help of laser induced fluorescence monitored the ions at room temperature and pressure up to 150 bar. Fulle et al. (1996) also used the laser induced fluorescence for the reunification of OH radicals. The maximum pressure and temperature were 150 bar and 700 K respectively. Sangwan et al. (2012) performed the experimental study of hydroxyl to hydroxyl reaction with the help of UV absorption monitoring technique at temperatures ranging from 296 K to 834 K and pressures ranging from 1 bar to 100 bar. Bahrami et al. (2012) performed the quantitative analysis of hydrogen peroxide. Brouwer et al. (1987) performed the theoretical calculations of reaction rates by using statistical adiabatic models. The temperature was in the range 200 K to 1500 K. Troe et al. (2008) used the ab-initio technique for the calculation of decomposition/recombination of H$_2$O$_2$ up to maximum temperature of 5000 K. This ab-initio technique is a quantum chemistry method and is a subject of computational chemistry (Levine 1991). Sellevag et al. (2009) used two transition state model for the calculation of rate constants with temperature ranging between 200 K and 3000 K.

Using shock tubes, Hong et al. (2009) conducted experiments regarding the H$_2$O$_2$ thermal decomposition. They used tunable laser absorption near 2.5 × 10$^{-6}$ m to detect the H$_2$O in the products. Hong et al. (2010) used IR absorption for the detection of H$_2$O at 2.55 × 10$^{-6}$ m in the temperature between 1000 K to 1200 K and pressure between 0.9 atm. to 3.2 atm. In another study, Hong et al. (2011) used UV absorption to monitor OH near 306.7 × 10$^{-9}$ m and used infrared absorption to monitor water near 2.55 × 10$^{-6}$ m. They measured the rate constant for hydrogen peroxide thermal decomposition at temperatures between 1020 to 1460 K and pressure at 1.8 atm. More recently, Sajid et al. (2013) performed the experiments for the analysis of thermal decomposition of H$_2$O$_2$ in a shock tube and used quantum cascade laser absorption near 7.7 × 10$^{-6}$ m. They performed the experiments in temperature range 930 – 1235 K and for pressures at 1, 2 and 10 atm.

As briefed above, most of the work in this area is experimental. On the other hand, Computational Fluid Dynamics (CFD) is a fast growing area to simulate the expensive physical experiments. Due to cheap availability of computers and state of the art softwares/tools which are both open source and freely available, it has become feasible to perform simulations in a rapid and cost effective manner. To harness the potential of CFD, the experimental setup described by Sajid et al. (2013) has been simulated in an open source OpenFOAM software. One of its solvers, reactingFoam has been used to perform the simulations using the limitedLinear and upwind convective