

# Detailed chemical kinetics model for thermal dissociation of UDMH

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Unsymmetrical dimethyl hydrazine (UDMH;  $(\text{CH}_3)_2\text{NNH}_2$ ) is one of the hydrazine derivatives used as a fuel of hypergolic rocket bipropellants. In the present study, we have developed detailed chemical kinetics model for thermal dissociation of UDMH. The rate coefficients for the UDMH decomposition,  $\text{UDMH} + \text{CH}_3$ ,  $\text{UDMH} + \text{NH}_2$ , and  $\text{UDMH} + \text{H}$  reactions were theoretically calculated for the present study by using quantum chemical calculations, i.e. CBS-QB3 and MRCISD+Q//CASPT2, and RRKM/master equation analysis. The other reactions were mainly referred from the previous models for monomethyl hydrazine,<sup>1</sup> hydrazine,<sup>2</sup> and dimethylamine,<sup>3</sup> and the H-C-N reaction kinetics from Dean and Bozzelli.<sup>4</sup> The resultant model consists from 65 species and 258 reactions, including Ar as a buffer gas. Figure 1 shows Arrhenius plot for the UDMH thermal dissociation reaction calculated at the initial UDMH concentration of 0.5 or 5% in the adiabatic and constant pressure conditions. The present model agreed qualitatively with the experimental results reported by Eberstein and Glassman,<sup>5</sup> and Just.<sup>6</sup> The sensitivity analysis suggested that the rate-limiting reaction at high temperature is  $(\text{CH}_3)_2\text{NNH}_2 (+\text{M}) \rightarrow \text{CH}_3\text{NCH}_3 + \text{NH}_2$ . At the lower temperature, the contribution of  $(\text{CH}_3)_2\text{NNH}_2 + \text{CH}_3 \rightarrow (\text{CH}_3)_2\text{NNH} + \text{CH}_4$  reaction is increased, and the overall dissociation rate comes to depend on the initial UDMH concentration.

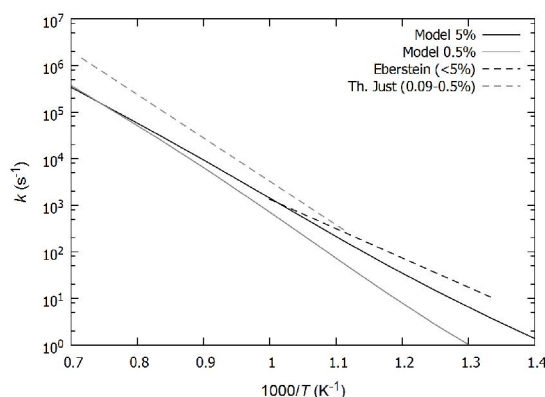


Fig. 1 Arrhenius plot for thermal dissociation reaction of UDMH.

## References

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