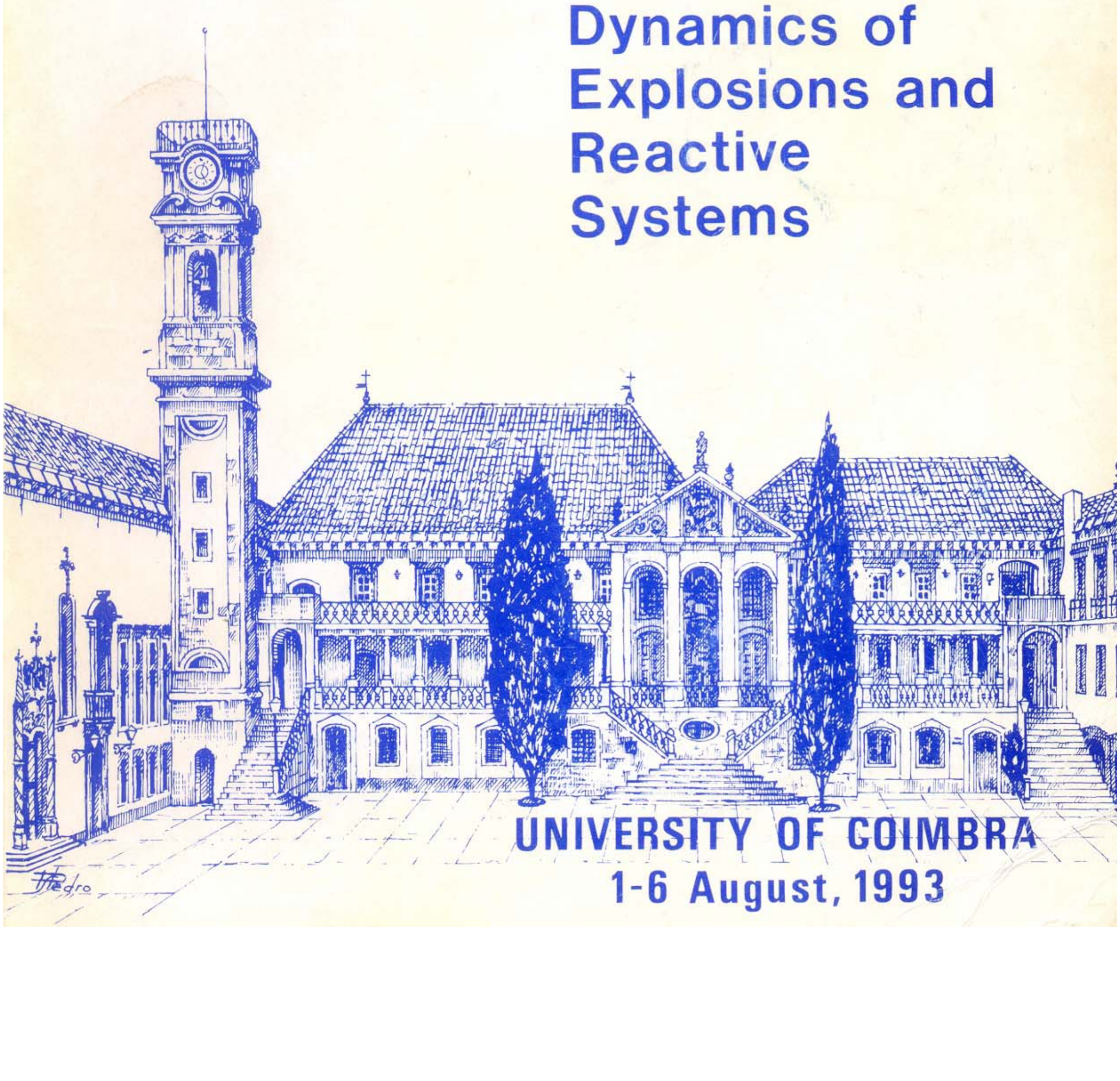
ICDERS

PREPRINTS
VOLUME II

14 th International Colloquium on Dynamics of Explosions and Reactive Systems



UNIVERSITY OF COIMBRA

1-6 August, 1993

Modeling of Detonability Limits for Hydrogen Mixtures

G.L. Agafonov, S.M. Frolov, B.E. Gelfand, A.Yu. Kusharin, O.E. Popov
N. Semenov Institute of Chemical Physics, Russian Academy of Sciences, Moscow, Russia

H.Gg. Wagner
Institute für Physikalische Chemie, Göttingen, Germany

Two models of detonability limits are suggested and studied, one of them is based on a simplified scheme of the reaction and the other uses the detailed kinetics. The models incorporate the physical mechanism of detonability limits, i.e. competition between the rate of chemical energy release in the reaction zone of a detonation wave and the rate of momentum and heat losses. Detonation fails when the losses dominate. The detona-tion limits are calculated for hydrogen-oxygen and hydrogen-air mixtures in ducts. The effect of mixture composition, inert diluents, initial pressure and temperature on the limiting detonation diameter is predicted. A comparison of the calcula-tions with numerous available experimental data shows that both models can be used for calculating detonability limits. The simplified model uses an empirical ignition delay correlations. Calculations performed for particular conditions agree fairly well with the parameters of realistic detonation waves. The detailed chemical reaction mechanism based on low-pressure reaction schemes yields significantly underestimated ignition delays. It was supplemented with reactions responsible for chain termination at high pressures, and the overall mechanism incorporating 42 elementary steps provided quantitatively adequate results for the detonability limits and their depen-dences on the initial pressure and temperature. Specific features of near-limit plane detonation wave structure were also studied and some important conclusions on the dependence of the reaction zone parameters on the initial pressure and mixture composition are drawn. The relations between the predicted reaction zone lengths, limiting tube diameters, and measured detonation cell sizes are established.