ACADEMIA ROMÂNĂ
SCOSAAR

Anexa nr.6

ABSTRACT

TITLE: Studies on deflagrations in gaseous mixtures

Habilitation domain: *Chemistry*

Author: VENERA GIURCAN

The habilitation thesis entitled ***Studies on deflgrations in gaseous mixtures*** describes the relevant scientific contributions of the candidate after obtaining a PhD in Chemistry at University of Bucharest, in 2008.

The manuscript is divided into three Sections: (I) Scientific, academic and professional achievements; (II) Career development plans; (III) References.

Section I includes an introductory chapter (Chapter I.1.) and five other chapters (Chapters I.2.-I.5.) in which the latest scientific results (based on 10 ISI representative articles, published as main author), and academic and professional achievements (Chapter I.6.) of the candidate are presented.

Chapter I.1. includes general information regarding the importance of the studied topics, the formation of gaseous mixtures with high explosive potential, the initiation and propagation of deflagrations in such mixtures, as well as the importance of using these mixtures in everyday life, and the parameters that characterize the propagation of deflagrations in such mixtures.

Chapters I.2.-I.5. describes in detail the main scientific achievements, addressing the following research directions:

- prediction of the flammability parameters (Chapter I.2.);
- laminar flames propagation in fuel-air-inert mixtures (Chapter I.3.);
- fuel-unconventional oxidant-inert flames (Chapter I.4.);
- explosion parameters of hydrogen-enriched fuel-air mixtures (Chapter I.5.).

In Chapter I.2., the prediction of the flammability parameters of fuel-air and fuel-inert gas mixtures in closed vessels is discussed. The study was carried out on mixtures with variable concentration of fuel and inert using explosion vesels of different shapes and volumes. CH_4, C_2H_6, C_3H_8, *n*-C_4H_{10} were used as fuels, and Ar, He, CO_2 and N_2 were used as inerts. The study allowed the

development of a new method for estimating the flammability range of fuel-air gas mixtures based on some explosion parameters obtained from experimental measurements (maximum explosion pressure and maximum rate of pressure increase). The peculiarity of this method is the use of these explosion parameters obtained in conditions far from the explosion limits. The proposed method for flammability hazards prediction can be used by any researcher working in the gaseous explosion field considering that this method do not require an expensive technique or a good expertise in this domain. It can be also used as screening preliminary protocol in recommending safety measures which are important in the use and handling of gaseous fuels. Part of the results of this study were obtained within the project PN-II-RU-PD-2011-3-0053, implemented in the period 2011-2013, entitled *Limiting conditions of explosion propagation in gaseous fuel-air and fuel-air-inert mixtures*, funded by UEFISCDI, and coordinated by the author of this thesis.

Chapter I.3. is dedicated to the study of flame propagation in fuel-air-inert mixtures. The purpose of this research direction was to examine the influence of adding an inert to fuel-air mixtures and to evaluate the explosion parameters that characterize the deflagrations produced in such mixtures. For this, experimental measurements were carried out in closed vessels with central ignition, as well as computations using specialized programs. Data were obtained at various temperatures, pressures and initial compositions, using ethane or propane as fuel, and N_2, Ar or CO_2 as inerts. The experimental and computed data obtained at the end of this research completed the scarce literature data in respect to flame propagation properties in fuel-air-inert mixtures, especially at initial pressures and temperatures different from ambient. Even though the study have been conducted using small-scale closed vessels, the results are considered useful for recommendations for fuel-air explosion mitigation occured at various initial pressures and temperatures in domestic or industrial plants taking into account that adequate safety protective measures can be formulated only on the basis of systematic studies concerning the characteristic parameters of deflagrations taking place in enclosures.

Chapter I.4. approaches the study of fuel-oxidant-inert flames when an unconventional oxidant (nitrous oxide - N_2O) is used. The study, carried out in closed explosion vessels, aimed to obtain the deflagration parameters of CH_4-N_2O-inert and C_2H_4-N_2O-inert mixtures (inert: N_2, Ar, He or CO_2) under different initial conditions (pressure, composition). The experimental results were supplemented and compared with results obtained from kinetic modelling that also provided detailed information about flame temperatures, concentrations of free radicals within the flame front or of the main compounds formed during combustion. The data obtained in this research share new perspectives

regarding the explosion phenomena when nitrous oxide is used as oxidizer since N_2O is more energetic compared with oxygen or air. On the other hand, the present results help develop explosion protection measures for handling, storage and use of these mixtures in industrial and domestic installations.

Chapter I.5. shows a study on fuel-air mixtures enriched with hydrogen. The research, also carried out in enclosures with central ignition and using various initial conditions, aimed to obtain and examine the deflagration parameters of these mixtures in order to improve the combustion properties of some commonly used fuels: LPG, butane, propane. In addition to the experimental measurements, calculations were also carried out using dedicated programs. The computed results were discussed in correlation with the rates of heat release and with the concentrations of the most abundant radical species in the flame front. The results showed that the addition of hydrogen to gaseous fuel-air mixtures leads to their burning velocities improvement, an important aspect in the design of burners or internal combustion engines.

The last chapter of Section I (Chapter I.6.) presents the main professional and academic achievements obtained by the candidate after obtaining the PhD title. Overall, 54 articles were published in ISI-listed journals (25 as main author), 5 papers in non-ISI journals (2 as main author), 3 papers published in proceedings (one as main author) and a book chapter. One of the projects undertaken and managed as director after obtaining the PhD title was financed by UEFISCDI. The other one is a bilateral project between Romania and Poland. Also, two mobility grants were obtained for participation in relevant conferences.

Section II presents career development plans conatinig details about ongoing research or the furure research directons that will be addressed.

In Section III, the bibliographic references corresponding to the presented content are listed.