FINAL REPORT
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BETWEEN
BROOKHAVEN SCIENCE ASSOCIATES
AND
E.I. DU PONT DE NEMOURS AND COMPANY

Project Entitled: Commercialization of Turbulent Combustion Code
CREBCOM for Chemical Industry Safety

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CRADA Final Report for IPP BNL-301

**“Commercialization of Turbulent Combustion Code CREBCOM
For Chemical Industry Safety”**

1. Introduction

A CRADA project was performed between BNL and DuPont de Nemours Co. (DuPont) of Texas under the auspices of IPP with the DOE support. The purpose was to jointly support Kurchatov Institute of Atomic Energy (Kurchatov) of Russia to develop the its CREBCOM (CRiteria and Experimentally Based COMbustion) code to the point where it could be commercialized and marketed for the special applications for the safety of chemical industry, as well as for general purpose combustion calculations. The work was performed from August 1, 2000 to March 31, 2008. The project resulted in improvement and validation of the CREBCOM code. The total cost of the sub-contract with Kurchatov was \$350,000, with matching fund from the industrial partner, DuPont.

2. Work performed

In the chemical process industry one often deals with explosive gaseous mixtures which under certain accident conditions can be ignited leading to catastrophic damage to the reactor and equipment in its direct proximity. An industry which has been plagued by accidental explosions leading to high collateral damage and loss of life is the off-shore gas drilling industry. As a response to these incidents, several explosion simulator codes were developed to analyze such explosions and to better design off-shore rigs to limit the damage from such explosions. These codes typically solve the Euler equations with a k- ϵ turbulence model and treat the flame front as flamelets which propagates at the local turbulent burning velocity. Since these codes were initially developed for simulating combustion phenomenon in highly vented open geometries, they are not designed to treat very fast flames and transition to detonation. Detonation is a supersonic mode of combustion which results in the highest pressure loading on structures, and thus the most damaging type of explosion. Due to the absence of a commercial code which has these capabilities, industries where these types of explosions are possible are forced to make simplifying assumptions concerning the initiation of a detonation.

This program developed the Kurchatov Institute's CREBCOM (CRiteria and Experimentally Based COMbustion) code to the point where it could be commercialized and marketed for the special applications described above, as well as for general purpose combustion calculations. The CREBCOM code uses a different approach to model the explosion phenomenon. The code models, with full 3D gas dynamics, the development of an explosion in three characteristics regimes: a) slow flames, b) fast flames, and c) detonation. The transition from one regime to another is governed by a set of empirical criteria and correlations. The advantages of CREBCOM over the standard explosion codes are:

- a) The CREBCOM code can predict the mutual effects of scale and mixture properties since the correlations used to predict the turbulent combustion velocity have scale included explicitly.
- b) The CREBCOM code is very fast, due to its efficient hydrodynamic solver and optimized numerical scheme. As a result, CREBCOM can be run on a standard desktop PC while existing codes must be run on a workstation or CRAY computer.
- c) CREBCOM is designed to predict transition to detonation and model detonation propagation

As part of the commercialization, the code was validated with the use of experimental data. The experimental data covered a range of thermodynamic initial conditions and apparatus scale. Proprietary experimental data were provided to the Kurchatov Institute by the DuPont for this purpose. The flame acceleration and detonation data was obtained from experiments in methane and oxygen enriched air mixtures carried out in two vessels with diameters of 20 and 27 cm. The experimental data covers a wide spectrum of initial temperature (20-525C) and pressure (1-3 atm). As part of this program, the Kurchatov Institute performed experiments in a 52 cm vessel in mixtures of methane-air at room temperature and pressure to be used in the validation of the code. The objective of these tests was to obtain flame acceleration data at a scale close to that found in actual industrial processes.

BNL was responsible for managing the DOE/IPP portion of the program, and for satisfying DOE reporting requirements. BNL also participated in an independent assessment of the CREBOM code.

DuPont provided proprietary experimental data to the Kurchatov Institute on flame acceleration and detonation in high temperature methane and oxygen enriched air mixtures in addition to the matching fund. In addition, DuPont also supplied to KI instrumentation for pressure and temperature measurement.

Kurchatov (KI) performed experiments at close to full-scale in mixtures of room temperature methane and air to develop the CREBCOM code which was used for explosion simulation in confined geometries, such as chemical reactors and converters. The code was validated by comparison of the code simulations with experimental data obtained under prototypic reactor mixture conditions.

Following tasks were performed during the project.

- Kick-off meeting was held in Russia. As part of the meeting, documents and information were exchanged and agreements between the parties covering matters such as confidentiality, intellectual property, and marketing rights were finalized. BNL and DuPont members visited the experimental facility.

- KI disclosed details on the current status and capabilities of the CREBCOM code. KI demonstrated convergence and robustness of the current version of the code via simulation of standard analytical problems.
- Setup of experimental apparatus, experiments started.
- Performance specifications and user-code interfacing (input and output) for the code were finalized.
- DuPont and BNL transferred proprietary experimental data to KI for simulation.
- Advanced development of CREBCOM code started where code components identified in the performance specifications were added or improved.
- Advanced development of CREBCOM code continued on user interfacing, i.e., make code user friendly for commercial use.
- Experiments completed and report summarizing data prepared
- KI carried out simulation of KI and DuPont sponsored experiments and discussed results with BNL and DuPont personnel.
- Code documentation was initiated.
- KI provided the final source code and operations manual to BNL and DuPont for independent assessment of the code.
- All parties met to review the status of CREBCOM development and validation using the experimental data.

3. Marketing

Kurchatov Institute has licensed a version of the code for application in Russia. Du Pont is responsible for marketing this code in USA.

4. Summary

Kurchatov - BNL – DuPont partnership developed the CREBCOM (CRiteria and Experimentally Based COMbustion) code to the point where it could be commercialized and marketed for the special applications for the safety of chemical industry. IPP funding helped provide jobs for a significant number of engineers and technicians that formerly worked on WMD.