12.5 Reactive Flow Simulation in Complex 3D Geometries Using the COM3D Code.

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Abstract

The COM3D code, under development at the Forschungszentrum Karlsruhe (FZK), is a 3-d CFD code to describe turbulent combustion phenomena in complex geometries. It is intended to be part of the advanced integral code system for containment analysis (INCA) which includes in addition GASFLOW for distribution calculations, V3D for slow combustion and DET3D for detonation analysis. COM3D uses a TVD-solver and optional models for turbulence, chemistry and thermodynamics. The hydrodynamic model considers mass, momentum and energy conservation. Advanced procedures were provided to facilitate grid-development for complex 3-d structures. COM3D was validated on experiments performed on different scales with generally good agreement for important physical quantities. The code was applied to combustion analysis of a large PWR. The initial conditions were obtained from a GASFLOW distribution analysis for a LOOP scenario. Results are presented concerning flame propagation and pressure evolution in the containment which clearly demonstrate the effects of internal structures, their influence on turbulence formation and consequences for local loads.

1. Introduction

In the case of a core melt accident in a Pressurized Water Reactor (PWR), considerable amounts of hydrogen may be generated, mainly due to the oxidation of the Zircalloy cladding. This poses a risk to containment integrity because hydrogen is easily transported through the compartments and can efficiently react with oxygen. In order to avoid fast combustion modes such as global detonation or turbulent deflagration, countermeasures are considered including the use of recombiners and igniters. Research is underway at FZK to improve understanding of the potential hazards and to support development and validation of hydrogen control systems.

The goal of the research activities is to provide numerical tools, based on validated mechanistic models, which allow to predict, on full plant scale, hydrogen specific phenomena which could occur in a severe core melt down accident in a PWR:

- hydrogen production, i.e. source rates and total amount.
- hydrogen distribution , i.e. local time dependent concentrations including the feedback of accident mitigation systems
- hydrogen combustion for the various modes, i.e. laminar and turbulent deflagration and detonation.

In addition, experiments are performed in geometries of varying complexity on different scales and under accident typical atmospheric conditions to provide the data base for the support of model development and code validation.

2. The Integral Code System INCA

The code system INCA (Integral Containment Analysis) consists of a family of codes each of which describes a specific physical process during the postulated accident:

- GASFLOW: distribution and transport of hydrogen and steam, including models for hydrogen mitigation (recombiners, igniters)
- V3D: slow combustion models, eg. the initial laminar deflagration, the transition to turbulent deflagration, and standing flames
- COM3D: fast turbulent combustion in partly or fully premixed atmospheres, including the regimes of corrugated flamelets, distributed reaction zones and well-stirred reaction
- DET3D: stable, fully developed detonation.

These specific numerical program modules are necessary because different space and time scales must be resolved in the different accident phases, and because the phenomena require different numerical schemes for the optimum solution, eg. implicit or explicit. The codes are written in a modular way and can reside on different computers. A central interface controls the evolution of the numerical simulation, switches between the modules according to appropriate criteria, and maps the variable fields from one module to the next, for instance, after ignition, from GASFLOW to V3D. The INCA system also contains options for input, post processing and on-line visualization.

3. The Combustion Code COM3D

3.1 Numerics

The COM3D code is a 3-d CFD code to describe turbulent combustion phenomena in complex geometries. It uses a TVD-solver, two turbulence models (standard k-ε and RNG k-ε), two chemistry models (Arrhenius for laminar and Eddy-Dissipation for turbulent combustion) and a multicomponent thermodynamic model which includes H2, O2, N2 and steam. The hydrodynamic model considers mass, momentum and energy conservation. Interfacing procedures were provided to facilitate grid-development in Cartesian coordinates for complex compartment and structure systems.

3.2 Code Validation

The hydrodynamic and thermodynamic models were verified against standard numerical test problems, e.g. Mach 3 flow against a forward facing step. Also, comparison to a FZK-tube test with a transient inert flow showed that turbulence formation is well predicted.

The COM3D reaction models were validated on combustion experiments peformed on different scales. In the 12 m tube at FZK, combustion tests were performed in obstacle geometry which increases turbulence formation. Fig. 1 (top) shows the calculational model for the tube, in which a series of rings provides for partial blocking of the open space. Various blocking ratios and hydrogen concentrations were investigated. Combustion is triggered at one end of the tube and pressure evolution and propagation of the flame front are detected with pressure transducers and light diodes. The comparison of calculated with experimental data shows good agreement for the acceleration phase (0 to 0.01 s) as well as for the final velocity for the incoming and for the reflected pressure wave.

In the 60 m RUT facility, combustion in more complex geometry including transmission from an obstructed channel to a large compartment was investigated (Fig. 2). Again, COM3D calculations reproduce well principal physical quantities like pressure evolution and flame speed.

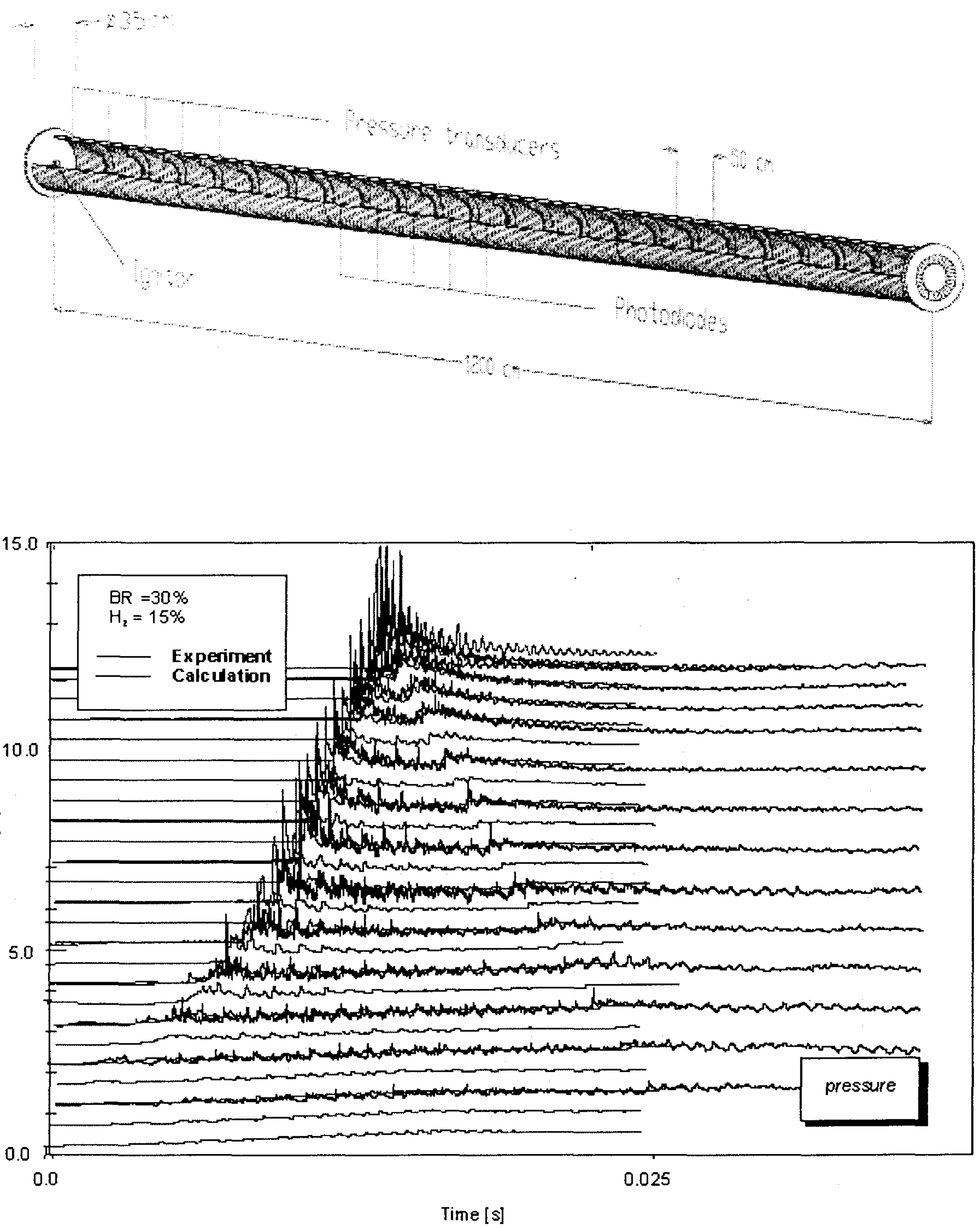
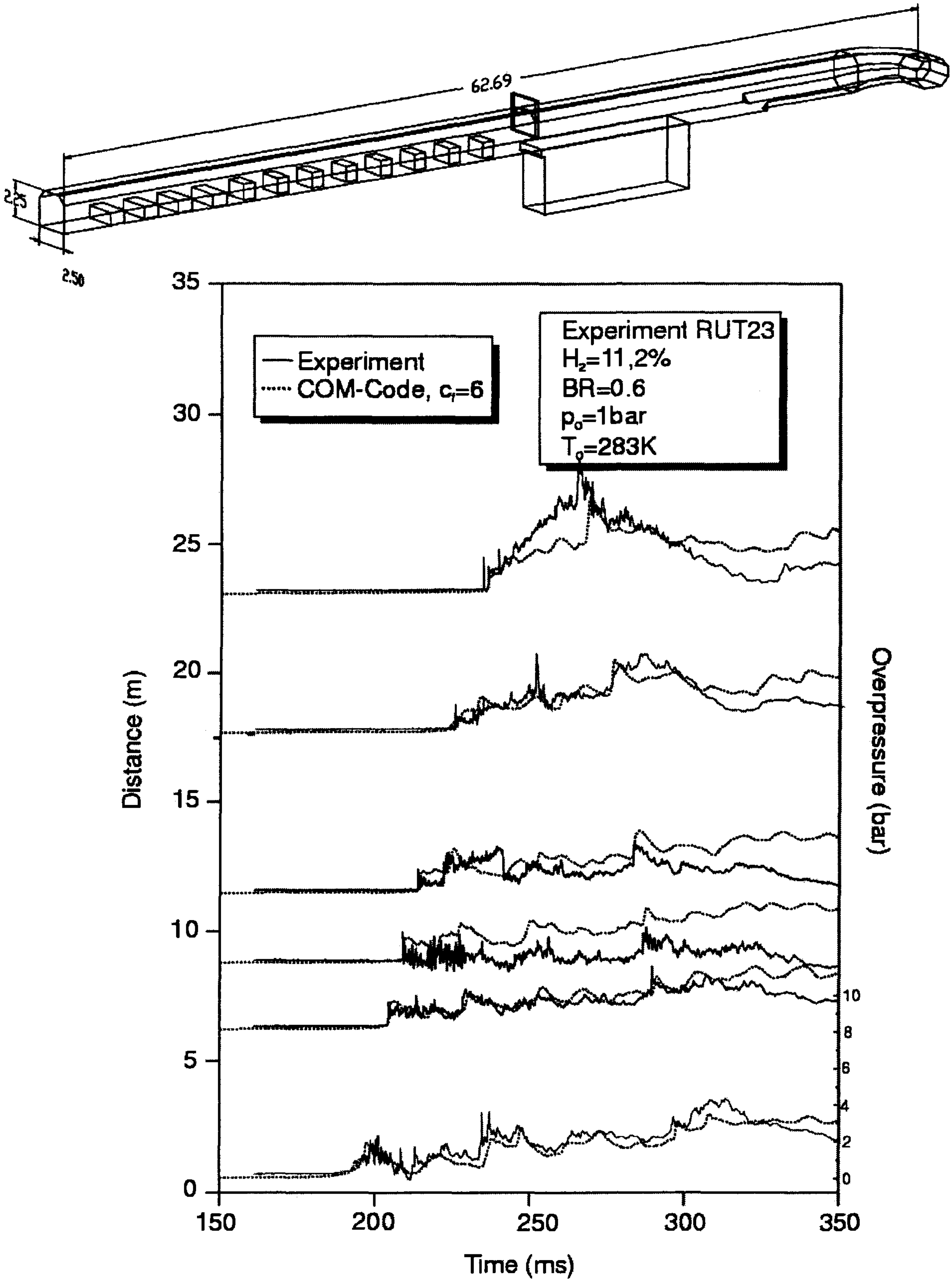


Fig. 1: 3-d view of FZK 12-m tube and comparison of measured and calculated pressure signals.



62.69
2.25
2.50
Experiment
COM-Code, c_f=6
Experiment RUT23
H_2=11,2%
BR=0.6
p_0=1bar
T_0=283K
Distance (m)
Overpressure (bar)
Time (ms)
0
5
10
15
20
25
30
35
150
200
250
300
350
0
2
4
6
8
10

3.3 Reactor Application

COM3D was applied to a full scale combustion analysis of a large PWR dry containment. The initial conditions were obtained from a GASFLOW distribution analysis for a LOOP scenario which resulted in a stratified atmosphere with dry hydrogen concentration of 9 to 13 % bottom to top. Ignition was triggered in one of the steam generator towers. Combustion progressed horizontally into the operating decks and upwards into the dome. It is interesting to note that the highest loads in terms of pressure are observed at the same horizontal level as the source and opposite to it. This is because turbulence formation is enhanced in the relatively small operating compartements and pressure waves superimpose at 180° to the source. Although H2 concentration is higher in the dome, the open space leads to less turbulence formation and therefore smaller loads.

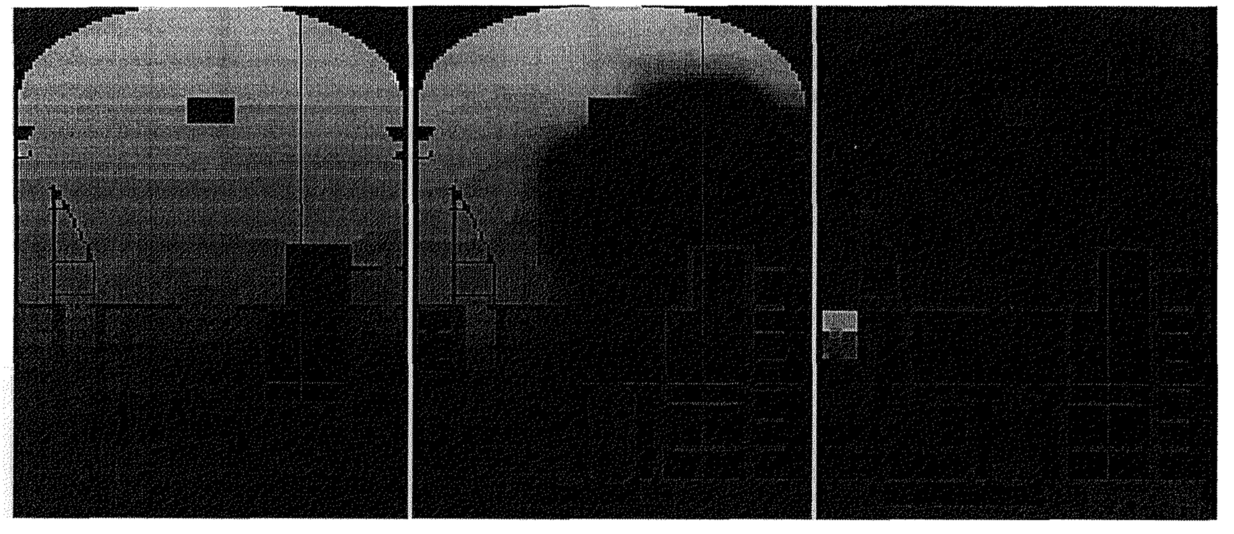


Fig. 3 a, b, c: Hydrogen concentration (a, b, 9 –13 %) and maximum pressure distribution (4 – 8 bar) in the containment. (Dark to light areas: low to high values).

4. Conclusions

The COM3D code for simulation of fast turbulent hydrogen combustion in large dry containments was developed. The mathematical, physical and numerical models for hydrodynamics, thermodynamics, turbulence and combustion were verified on standard test problems and experiments on different scales. The combustion tests covered reactor relevant scales (60 m).

The verified models were applied to the analysis of a full scale containment burn in a potential future reactor design. The progress of the combustion in the initiallly inhomogeneous H_2-distribution was largely determined by local turbulence generation in the complex compartment geometry. The expansion of the burned gas produced gas velocities of the order of 100 m/s. The highest local dynamic loads reached about two times the AICC pressure of the average mixture. They occured by superposition of flame fronts opposite to the ignition location.

This test demonstrates the feasability of full scale combustion calculations for NPP analysis under severe accident conditions.