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# Validation of GASFLOW for analysis of steam/hydrogen transport and combustion processes in nuclear reactor containments

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ABSTRACT: A steam/hydrogen transport test in a large containment geometry and different 3D hydrogen combustion tests were analysed with the GASFLOW code. Results broaden the validation basis to simulate accidental hydrogen release and combustion in reactor containments in a 3D finite volume approach.

## 1. INTRODUCTION

Steam and hydrogen release into a light water reactor containment may occur during a core melt down accident. Without hydrogen countermeasures, this event could lead to high pressure and temperature loads due to combustion. Safety regulations require the demonstration that such loads don't pose a threat to the containment structure. The GASFLOW code developed at Los Alamos National Laboratory (LANL) is one important tool for an integral description of the related transport and combustion phenomena. A cooperation agreement between LANL and Forschungszentrum Karlsruhe (FZK) gave FZK access to GASFLOW in exchange for experimental data from German government funded programs in the Heißdampfreaktor (HDR) and in the Battelle model containment (BMC). GASFLOW is being developed at FZK for the integral analysis of steam/hydrogen transport with the impact from hydrogen recombiners and combustion due to ignitors on the convection process. FZK work with GASFLOW has focused on the validation of relevant models for transport and combustion and on the testing of its integral analysis capability. This paper summarizes the results from the containment related GASFLOW validations, that have been jointly performed with LANL.

## 2. OVERVIEW OF THE GASFLOW CODE

GASFLOW is a 3D finite-volume computer code (Travis) that solves the time-dependent, compressible Navier-Stokes equations for multiple gas species. The fluid-dynamics algorithm is coupled to the chemical kinetics of combusting liquids or gases to simulate diffusion or propagating flames in complex geometries of nuclear containments. Modeling includes the energy release and mass diffusion at catalytic recombiners and their contribution to the fluid convection. Fluid turbulence is calculated to enhance the transport and mixing of gases. Condensation and heat transfer to walls and internal structures are calculated to model the appropriate energy sinks. Wall surface temperatures are calculated using small surface nodes in a transient, 1D heat conduction model with a variable mesh. The solution procedure of the governing equations is a modified Los Alamos ICE'd-ALE methodology.

## 3. TESTS FOR HYDROGEN/STEAM TRANSPORT

The condensation model in GASFLOW has been validated with a 3D analysis of the containment thermohydraulics of the Phebus test vessel (Hardt). The Phebus experiments analysed were from four constant steam injection rates of the pre-test series and the varying steam and hydrogen injections in test FPT0. Steam condensation in these tests occurred only on the surface of 3 "wet" condenser rods attached below the head of a 10m**3 vessel with 120 degrees symmetry. These rods were cooled and maintained at a controled surface temperature, while the remaining surfaces were heated just enough to prevent condensation. Due to the defined wall temperatures, the con-

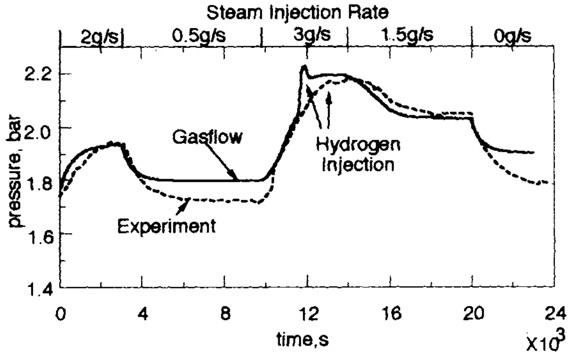

Fig.1: Containment pressure in Phebus test FPT0

densation model, which was derived from a Reynolds analogy, could be tested without influences from heat conduction. The calculated pressure variations for different steam and hydrogen injection rates show good agreement with the experiments. Analysis of the 5 tests used the same mass transfer coefficient that was calibrated from one experiment. A condensation enhancement function is applied when large steam volume fractions are present (Royl). The analysis demonstrates the need to apply 3D models to capture the complex flow patterns. GASFLOW predicts the pressure increases quite well during large steam injections in test FPT0. The pressure reduction at reduced steam injections and the increase during hydrogen injection are calculated with too little steam diffusion to the condensers. This explains higher GASFLOW pressures in these phases (Fig. 1).

Starting from previous work (Lam) a re-analysis of the HDR test T31.5 (Cron) was made after validating the condensation model with the Phebus tests. Test T31.5 simulated the steam and hydrogen release after a large break Loss Of Coolant Accident (LOCA) in a 50m high, 20 m diameter, steel shell containment with a free gas volume of 11,000 m**3 . The re-analysis uses a finer 3D finite volume discretization with 11 radial, 24 azimuthal and 40 axial cells. A new liquid water film tracking model allows vaporization of condensed films thus cooling structures during rapid pressure reductions . A homogeneous equilibrium two phase model (HEM) was added. The HEM simulates bulk vaporization due to flashing of the injected water and it allows bulk condensation when steam oversaturates. A parametric "rain-out" model is applied for water removal. The calculated pressure (Fig. 2) agrees well with the test data, particularly in the final phase. It displays a rise and decay during and after the initial blow down and a temporary halt of the decay during the second steam injection phase at 23 min. After 36 min it shows a slight increase during the 12 min injection period of the light gas (LG=H2 simulated with 85%He and 15%H2). Good agreement is obtained for the temperatures in the dome and near the breakroom. Exact overflow opening areas are modeled by introducing a fractional mesh area at more than 94 locations. This effectively changes the direction of natural circulation so that upflow goes through the spiral stair case and downflow in the main stair case, which is in

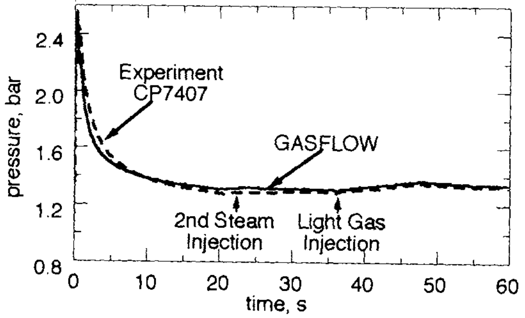

Fig. 2:Containment pressure in HDR Test T31.5

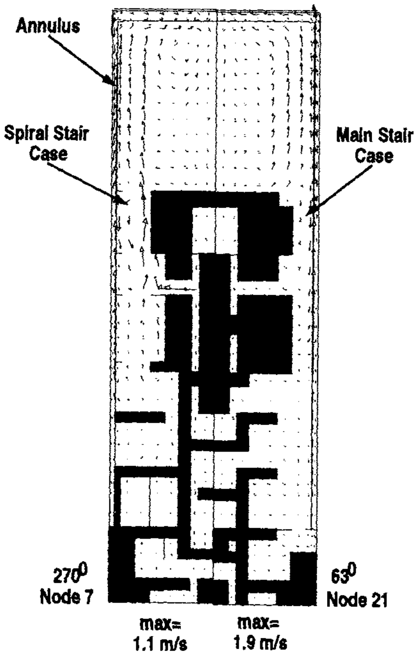

Fig. 3: Main circulation paths during light gas injection in HDR test T31.5 at 2200 s

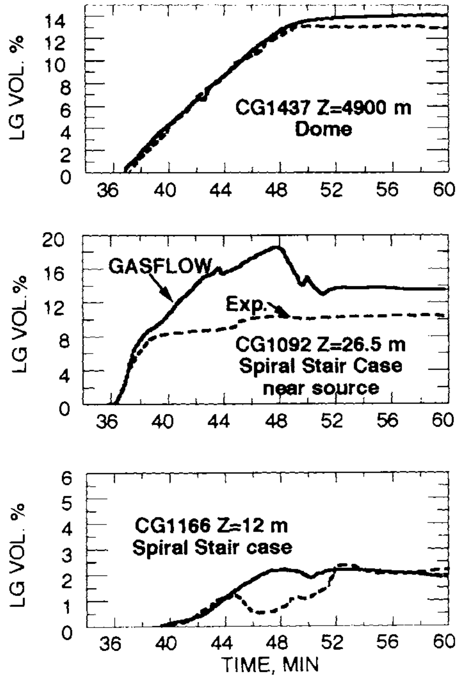

Fig. 4: Light gas distribution in test T31.5

agreement with the experiment (Fig.3). LG is then released with the correct circulation. The LG distribution (Fig. 4) matches the test data better than the results from any other published analysis of this experiment. The stratification of LG in the dome is particularly well captured. The differences near the source location occur in regions with steep gradients. There the sensor locations are slightly off in the discrete GASFLOW mesh.

If the 14% LG in the dome were hydrogen, this mixture could combust. To test the integral analysis capability GASFLOW simulated a 3D combustion process in the entire HDR containment at the end of the transport analysis. The calculated light gas distribution from test T31.5 was interpreted as hydrogen and ignited in the top centre of the dome. The flame front propagates downward against gravity. It requires more than 450 ms to reach the level of the stair cases. But then the flame moves rapidly towards the source location through the stairs. The flame propagation is shown by the outward velocity vectors below the contour plot of the hydrogen volume fractions (Fig. 5). A peak pressure of 8 bar is calculated. It then levels off at 4 bar after the combustion. Gas temperatures reached 1500K one sec after the ignition. While the 60 min transport analysis with 12300 computational cells took about 12 h of Cray YMP time, GASFLOW cal culated the final 3D combustion process in less than a minute.

## 4. TESTS WITH HYDROGEN DEFLAGRATION

To validate the combustion model in GASFLOW, we analysed selected tests from the HDR E12 and BMC HX series.The combustion simulations applied new higher order temperature approximations for the internal energy and the specific heat of the gas mixtures and for the molecular transport properties fitted to data from the JANAF tables and the Chemkin code, respectively (Müller). Turbulent diffusion was simulated using the algebraic model.

The HDR E12 series was performed in two sealed off rooms within the HDR containment (Rastogi). One room was more horizontal with 200 m**3, while the other room was more vertical with 330 m**3 . The rooms were connected through an orifice with an obstacle near the opening. The large vertical room could vent into the containment after failure of a rupture foil. The two volumes were simulated in a 3D cartesian mesh with 51 x 27 horizontal and 35 vertical cells, an additional 13 vertical cells were used for the expansion volume. The rooms were filled with a mixture of air, about 12% H2 and 25% steam. The selected three tests used rather similar mixtures

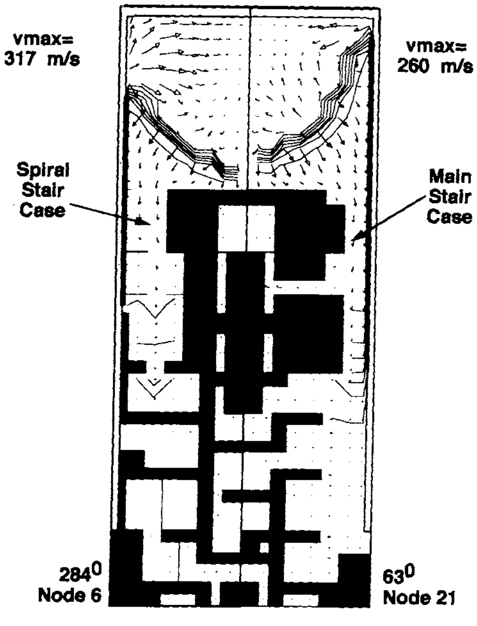

Fig. 5: Flame front from H2 burn 450 ms after ignition in T31.5 geometry

but different ignitor positions.

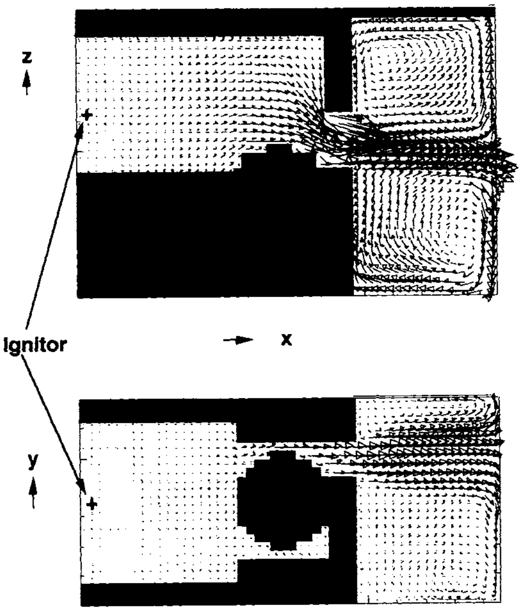

Fig. 6: Jet ignition in 3D GASFLOW analysis of HDR Test E12.3.3 (2.3 s)

Test E12.3.3 examined a horizontal accelerated hydrogen jet deflagration in a subcompartment chain with the ignition at the far end of the room. GASFLOW predicts the jet ignition behind the opening from the horizontal to the vertical room rather well. The flow distribution in Fig. 6 is taken at 2.3 s after the ignition. It is strongly 3 dimensional and has a maximum velocity of 236 m/s. GASFLOW somewhat overpredicts the measured peak pressure of 1.8 bar (Fig. 7). The time scale of the analysis required a time shift of 0.75s to match the occurrence time of the peak pressure. Such time shifts in combustion simulations are common because the development of a sustained flame after the ignition depends on local initial conditions that are unknown. GASFLOW burns nearly all the hydrogen. Hand calculations show that the calculated pressures finally oscillate around the adiabatic isochoric complete combustion (AICC) limit for the full expansion volume. The simulated heat exchange with the walls is negligible on this time scale. Due to the lower final test pressure overall less hydrogen must be in the system or more hydrogen must have escaped to the upper containment without combusting. Mass balances before and after the test don't resolve these discrepancies. Test E12.2.2 examined a horizontally oriented deflagration with ignition close to the opening connecting the horizontal with the larger compartment. A slower bi-directional horizontal flame expansion is calculated without jet ignition. The peak pressure is reduced by 0.8 bar, and it approaches the same AICC pressure. The test data confirm this tendency. But the peak and final test pressures are somewhat lower than calculated. The hydrogen inventory again is not well known. Test E12.1.2 involved a vertical hydrogen deflagration in the larger compartment with the igniter location low in the same room. GASFLOW predicts a similar peak pressure as in E12.2.2 for the same gas mixture. The flame velocity remains small, where jet ignition into the horizontal compartment has little or no effect. This is qualitatively in agreement with the test data, but this calculation suffers from larger uncertainties because the measured hydrogen distribution and overall mass concentrations exhibit significant and unknown local variations.

Analysis of deflagrations with jet ignition was also performed for three H2-air combustion tests in the Battelle model containment (BMC). We investigated 9 to 10%H2-air

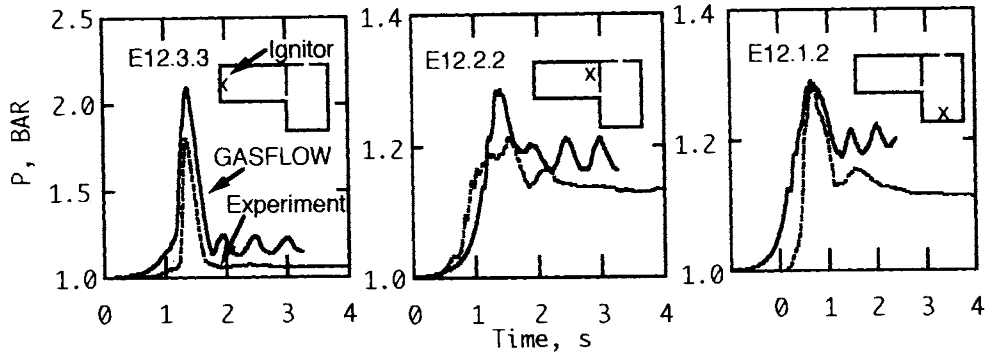

Fig. 7: Combustion pressures in tests from the HDR E12 series with different ignitor positions (mixture of air with 12% H2, 25% steam)

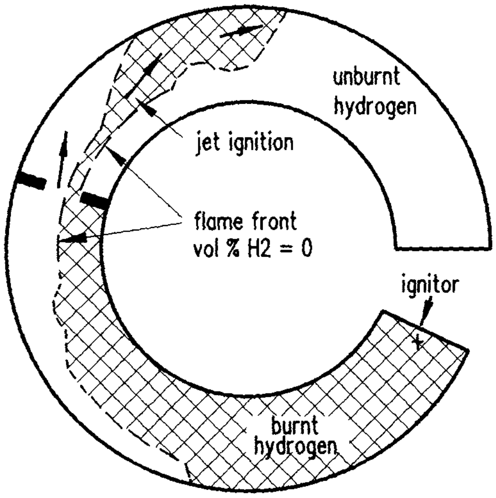

Fig.8: Flame front in BMC test HX14 with 2 ring rooms in axially centred r-Θ plane at 2.4 s

mixtures in BMC tests HX14, HX12, and HX23. These tests involved 2, 3, and 4 chain-type connected rooms, respectively. Venting into a larger dome volume occurred after failure of a rupture foil (Kanzleiter). Combustion in the banana shaped rooms (each of 41m**3) was simulated by 3D models. Each calculation showed significant centrifugal effects which couldn't be captured in earlier simulations that were restricted to 2D models. Typically the flame front moves from the inner towards the outer radius while progressing through the rooms. (for example Fig. 8, the 2 room test HX14 at 2.4s). The centrifugal effects become more dominant for higher velocities during jet ignitions down stream of narrow openings. Complicated multiple flame fronts and gas pockets develop. Test HX23 was a four room test in which two flame propagation regions developed. GASFLOW confirms the finding of weaker jet ignitions for cross flow vs. longitudinal flow enhancement at openings. Flame fronts develop in the upper and lower room chain (Fig. 9) and then converge near the exit to the dome. Test results indicate a pressure enhancement when the flame fronts meet. GASFLOW underpredicts this phenomenon (Fig. 10). The pressure increase is rather sensitive to details of the ignition process. Ignition in the last room occurs twice as each flame front arrives. The incoherency between these two ignitions controls the height of the pressure peak and also the amount of unburnt gas that can escape to the dome. Different flame running times probably result from unresolved local effects around the ignitor in the first room. Pressure levels are lower than the measured values which indicates that less gas has been burnt. For the other BMC tests, final GASFLOW pressures are near the test data. In test HX14 involving two rooms, good agreement is obtained for the pressure peak, only the first small peak at failure of the rupture disk is not calculated. Test HX12 with three rooms has subsequent jet ignitions from cross and longitudinal flows. The calculated pressure in the middle room doesn't quite peak at the test data. The combus tion time is extended in the GASFLOW calculation.

## 5. CONCLUSIONS

With the newly implemented models for the transport and combustion simulations, GASFLOW performs quite well in the analysis of selected tests. The predictive quality is expected to improve as experience with the code accumulates. Integral analysis of

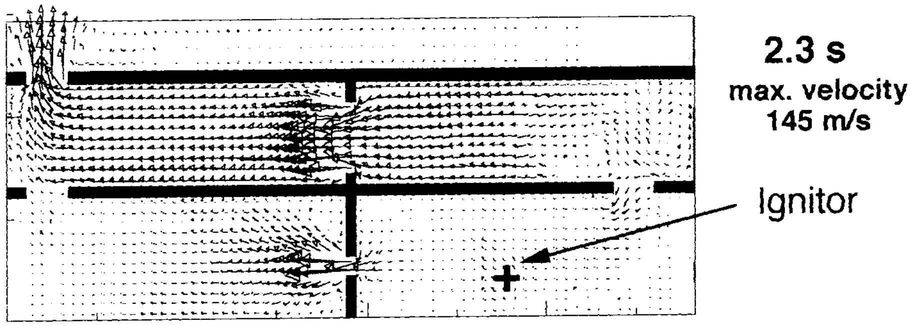

Fig. 9: Velocity field in radially centred z-Θ plane during BMC test HX23 with 4 ring rooms

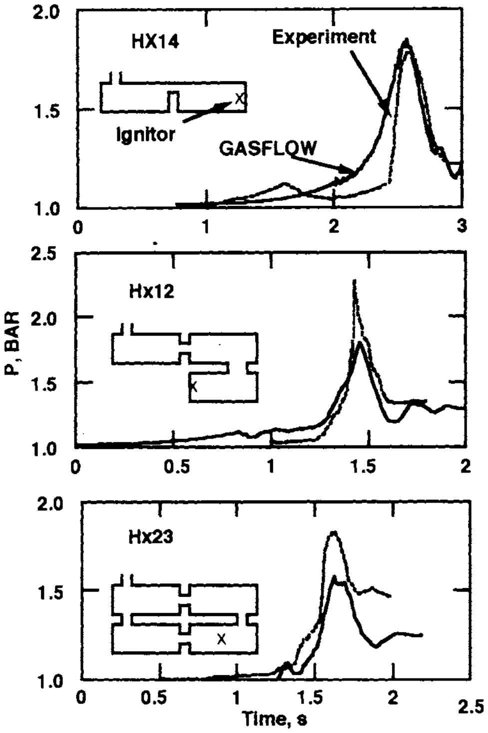

Fig. 10: Pressures in BMC tests with 2, 3, and 4 room chains

transport and combustion sequences have been demonstrated, additional validation work will continue in this area. One key problem for transport analysis is currently the running time, which can be long for complex 3D problems. The validation effort is continuing with analysis of the HDR test E11.2 using the same model as in T31.5. Validations will also include experiments involving hydrogen recombiners. The objective is to qualify GASFLOW as a validated integral tool for the analysis of steam/hydrogen transport and combustion processes. GASFLOW will provide a mechanistic simulation, and eventually become one design tool to analyse various mitigating features for hydrogen releases and subsequent combustion loads that will be considered for the development of new reactor containments.

## 6. ACKNOWLEDGEMENTS

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