6.4 CALCULATIONS CONCERNING THE CAPABILITY OF PASSIVE RECOMBINERS TO CONTROL HYDROGEN CONCENTRATION IN THE CONTAINMENT OF AN ADVANCED PWR

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Abstract

The Department of Mechanical and Nuclear Constructions of the University of Pisa has developed a computer code, HOCRA, which is able to make an initial evaluation of the capability of catalytic recombiners to remove hydrogen from the atmosphere of the safety containments of nuclear reactors in accident conditions. The code allows the analysis of the average concentration transient of hydrogen in a generic compartment of a safety containment in a nuclear reactor. The software is structured into two groups. The first, mode-1, analyses the average concentration in all the free volume of the containment before a possible venting; whereas the second, mode-2, analyses the average concentration transient in a containment compartment, assuming input and output flow rates into and from the compartment itself. The first part of this paper outlines the physical and mathematical model of the code, the second part reports calculations made for an advanced PWR in cooperation with ENEL.

1. Introduction

Combustion cannot propagate in a gas mixture of fuel and oxidizer if at least one of the two reactants is below its flammability limit. In order to maintain the containment atmosphere non-flammable during an accident in a nuclear reactor, hydrogen and oxygen can be recombined with thermal or catalytic devices.

Recombining means that H_2 and O_2 can react significantly even at low temperatures and non-flammable concentrations, but in any case much more slowly than in a deflagration, so that the energy production rate is lower and cannot substantially affect the pressure in the containment. On the other hand, for the same reason, recombining cannot in itself cope with a high hydrogen discharge rate.

If, in spite of this mitigation system, the gas mixture composition goes over the flammability limits, recombining may also be useful for avoiding strong explosions.

Recombiners can increase the chances of success of deliberate ignition, by reducing the number and size of possible pockets of more reactive mixtures and by limiting ignitor location to the zones where it is more likely that H_2 concentration increases too fast to be controlled by recombining.

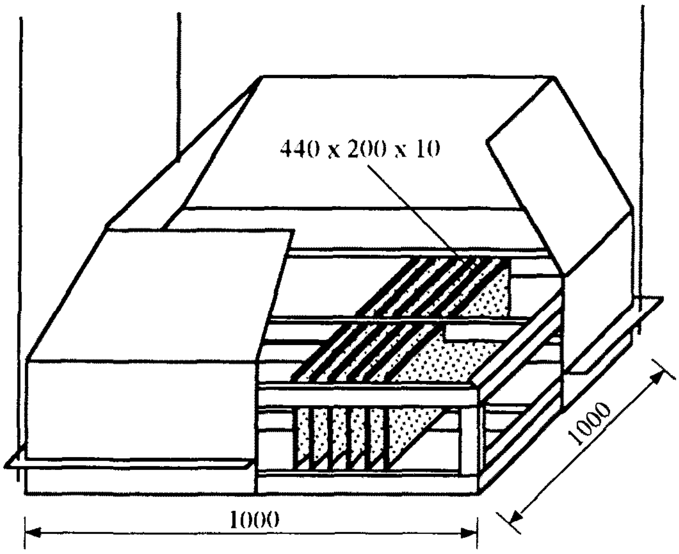

Figure 1. NIS catalytic recombiner

The new passive autocatalytic recombiners (PARs) that are currently being marketed by the NIS Company, Fig. 1, and Siemens ('small', 'medium', and 'large' types), Fig. 2, are simple and reliable devices without moving parts and require no source of power. They can begin to remove hydrogen before flammable conditions are reached, also when the environment is inerted by steam.

Tests also highlighted that the working of the PAR is not substantially altered by the presence in the atmosphere of poisons or common catalytic inhibitors (aerosols, liquid drops, iodine, carbon monoxide) since the catalyst is never completely deactivated, even if exposed for several days, and the temperature reached by the catalyst has a "self-cleaning" effect. The recombiner seems to reach the steady-state quite rapidly, especially if the catalyst is coated with a water-repellent film.

PARs seem to be able to cope with higher generation rates of hydrogen better than the old active thermal recombiners, because more units can be installed at the same cost and in the same space.

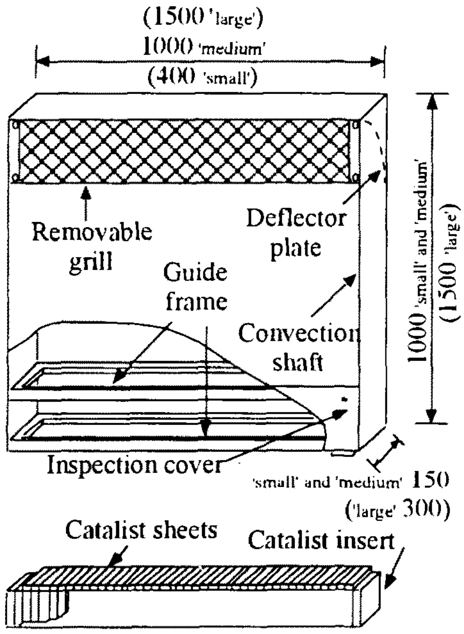

Figure 2. Siemens catalytic recombiner

Nevertheless, there is still some concern about their behavior in particular conditions typical for severe accident and/or for containment compartments. There are some difficulties in sizing the hydrogen control system and, in particular, in determining the PAR number and location for specific plant designs. To solve them by analysis, it is necessary to develop appropriate tools able to simulate the PAR operation and performances in the actual primary containment accident conditions. It is important to note that these conditions are different from the conditions in which the PARs are normally tested.

Empirical correlations were written by the Department of Mechanical and Nuclear Constructions of the University of Pisa in the framework of the European H2 Project (1992-1995) [1-3], to evaluate the capability of the catalytic recombiners. On the basis of these correlations, a computer code, called HOCRA (HOmogeneous Condition Recombiner Assessment), has been created to calculate the decrease in H_2 concentration due to any number of recombiners which are installed in a volume where the balance is known between inflow and outflow rates of all the different gas components. In cooperation with ENEL, which is the national electricity board in Italy, some calculations were carried out to verify the possibility of controlling the hydrogen concentration with PARs in an advanced PWR containment during severe accident scenarios.

2. The mathematical model

In order to evaluate the average concentration transient of hydrogen in a given volume in the presence of catalytic recombiners, the physical and chemical processes that take place in the catalytic oxidization of H_2 need to be defined, along with the quantities that influence the phenomenon and the correlation between these quantities and the overall recombination rate. In fact, it will thus be possible to correctly formulate the system of differential equations (balances of mass, momentum, and energy), and by integrating these the evolution of the phenomenon in time will be given.

2.1. The recombination rate

The gas that flows through a passive recombiner is heated due to the exothermic H_2-O_2 reaction that takes place within. The increase in temperature and thus the change in gas density depend on the quantity of hydrogen that recombines in the unit of time (recombination rate), which represents the heat source, and on the cooling capacity of the gas that passes through the recombiner. The driving pressure due to the difference in density between the inside and the outside must be counterbalanced by the pressure loss of the gas in the recombiner, due to friction and the increase in kinetic energy in the gas.

The power generated by the recombiner influences the circulation of air in the environment where the recombiner is located, which also depends on the geometry of the environment, on the location of the recombiner, and on the natural and forced convection due to any other cause.

In feedback, this circulation then affects the power from the recombiner because it affects the thermal-hydraulic conditions of the inlet gas, on which the working of the recombiner depends; specifically, the velocity, pressure, temperature, and chemical composition.

A complete and reliable simulation of the behavior of a recombiner inside the safety containment of a nuclear reactor can thus only be made by joining two models together:

- the first, or 'external' model, expresses the variation in the thermal-hydraulic conditions of the gas while it flows throughout in the environment where the recombiner is located, after it has left the recombiner and before going back into the recombiner itself

- the second, or 'internal' model, expresses the change that the same quantities inside the recombiner undergo

The current models [4-10] do not totally satisfy these requirements.

The problem can be considerably simplified if the volume where the recombiner is located is perfectly stirred. In this case a unique empirical correlation can link the recombination rate to the thermodynamic conditions in the volume.

Quasi-steady-state recombination rates were evaluated by the recombiner manufacturers on the basis of experimental tests [4-5]. They are supplied as empirical functions of the volumetric concentration of hydrogen and of the pressure in the volumes where the recombiners were installed during the tests. These evaluations of the recombination rate of passive recombiners are based on experimental data of decreases in hydrogen concentration, obtained during recombiner operations in relatively small volumes. The composition of the gas mixture was almost uniform in the test vessels, because of the convective flow generated by the recombiner itself.

An analysis of these empirical functions showed that the recombination rate (R_r) might only be, although very roughly, proportional to the molar density of the deficiency reactant (hydrogen in the tests), Fig. 3 [8], and so be practically independent of pressure, temperature and inert gas concentration.

The correlation chosen in HOCRA to connect R_r to the experimental variation of $[H_2]$ is the following function:

$$R_r = A\,[H_2]^C \qquad (1)$$

where A and C are the constants, whose values are derived from a best fit of the experimental data (Fig. 3) and differ depending on the type of recombiner (NIS, Siemens large, medium or small).

In advanced PWRs, the free volume in the safety containment is such that, even if a hydrogen mass is considered that would be produced by the oxidation of all the zirconium contained in the reactor core, the average composition of the mixture in all the containment would still be hypostoichiometric. On the other hand, in the individual compartments of the containment, transient atmospheres may be verified with a hyperstoichiometric H_2 concentration.

Hyperstoichiometric mixture conditions were not sufficiently tested, but it is reasonable to assume that the recombination rate is influenced by the average molar density of O_2. In order to estimate the removal rate of H_2 even in hyperstoichiometric mixture situations, it was assumed that the recombination rate is connected in all conditions to the molar density of burnable H_2 ($= [H_2]$ for hypostoichiometric mixtures and $= 2\,[O_2]$ for hyperstoichiometric mixtures). Under this hypothesis, in the hyperstoichiometric field, correlation (1) becomes:

$$R_r = A\,(2[O_2])^C \qquad (2)$$

where A and C have the same values as in the hypostoichiometric case.

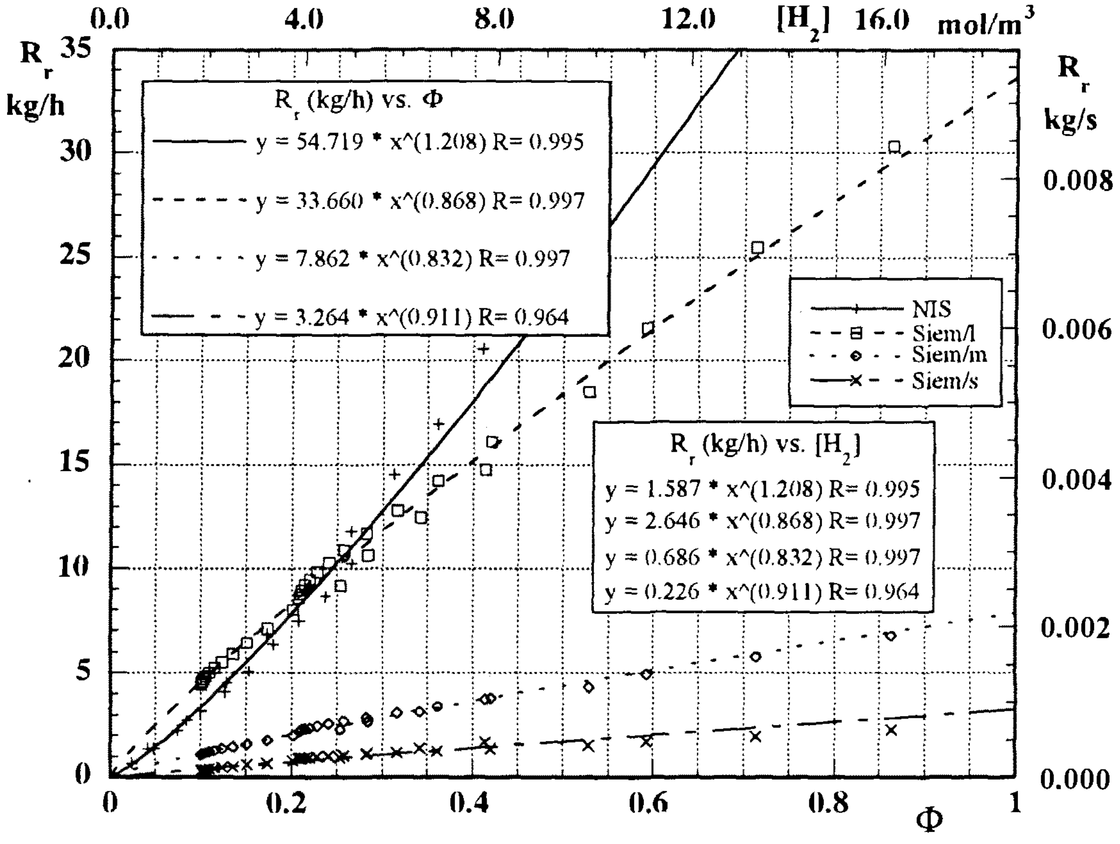

Figure 3. Recombination rate vs. [H$_2$] in a stirred environment

2.2 HOCRA mode-1: uniform mixture in the containment

In a volume in which the thermodynamic conditions are assumed to be uniform, which may also result from the action of the recombiners which facilitate mixing within the containment, the study of the concentration transients of hydrogen and oxygen can be approached using the following mass balances:

$$\frac{d[H_2]}{dt} = \frac{J_{i,H_2} - J_{o,H_2}}{V_t} - \frac{N_t}{V_t}\frac{R_r}{M_{H_2}} \qquad (3)$$

$$\frac{d[O_2]}{dt} = \frac{J_{i,O_2} - J_{o,O_2}}{V_t} - \frac{N_t}{V_t}\frac{R_r}{2M_{H_2}} \qquad (4)$$

This situation is assumed by HOCRA mode-1 for the whole free volume of the safety containment of a nuclear reactor before venting. In order to calculate the average transient concentration of hydrogen, it thus requires only knowledge of the hydrogen release rate in the accident situation, in so far as the containment is closed and the oxygen release due to radiolysis may be neglected ($J_{i,O_2} = J_{o,H_2} = J_{o,O_2} = 0$). The hydrogen release rate can be derived by containment codes.

2.3 HOCRA mode-2: non-uniformity conditions

HOCRA mode-2 evaluates the average hydrogen concentration in a volume where, although the temperature and concentrations are not uniform, they nevertheless allow a subdivision into sub-volumes, each of which is perfectly mixed. In a nuclear reactor containment, the sub-volumes may reflect the physical compartments of the containment, but more generally, they define the areas in which the thermodynamic coordinates of the mixture can be considered uniform.

The H_2 and O_2 transients in a sub-volume are still described by equations (3) and (4) where now all the quantities concern that sub-volume.

The change of the average H_2 molar density in the containment is then given by the following:

$$\frac{d[H_2]}{dt} = \frac{J_{i,H_2,t} - J_{o,H_2,t}}{V_t} - \frac{1}{V_t M_{H_2}} \sum_{j=1}^{NVI} N_j R_{r_j} \qquad (5)$$

where the index t refers to the overall conditions (with reference to the total volume V_t), whereas j refers to the j-th of the NVI sub-volumes in which V_t is divided.

HOCRA mode-1 would give a correct assessment of the $[H_2]$ transient, even if the thermodynamic conditions in the containment volume were not uniform, only if (i) the type and spatial distribution of the recombiners were the same in all the volume, (ii) the exponent C in correlations (1) or (2) were equal to 1, and (iii) the mixture were hypostoichiometric, or hyperstoichiometric, in the whole volume.

Since the recombination rate of the recombiners currently on the market is simulated in HOCRA with a power function in which the exponent $C \approx 1$ (Fig. 3), the results obtained with HOCRA mode-1 could in many cases be a good estimation of the real variation of $[H_2]$ in time.

The presence of recombiners in a compartment, in addition to the thermodynamic condition of the mixture in the volume, also influences the mass (and energy) exchanges with the neighboring compartments. Thus a correct simulation can only be given by implementing a complete mathematical model of the recombiner in a containment code.

In HOCRA mode-2, the difference between the inlet and outlet flow rates is derived from the transients of pressure, temperature, and molar fractions of hydrogen and steam calculated by other codes in the absence of recombiners. This means that the balance between the entering and exiting flows into and from the volume are assumed the same both in the absence and presence of recombiners, or that the thermal-hydraulic exchanges between neighboring compartments are assumed to be not affected by the variations in energy and chemical composition due to the recombination. This hypothesis is actually untrue but is useful for an initial evaluation of the capability of the recombiners. The difference between the inlet and outlet flow rates is considered to be constant between two successive points of sampling, thus some peaks might be smoothed out in this time interval, if sampling is not sufficiently frequent.

Table 1 - Accident conditions

CASE	HYD1	HYD2	HYD3
Sequence	2" Hot Leg Break	4" Hot Leg Break	Transient (loss of feedwater)
System ⇓	**Status**		
Accumulators	Yes (1 on 2)	Yes (2 on 2)	Yes (2 on 2)
Core makeup tanks	Yes (2 on 2)	No	Yes (2 on 2)
ADS	Yes (stages 1, 2, 3)	No	Yes (stages 1, 2, 3)
IRWST in vessel injection	Yes (at vessel failure)	Yes (at vessel failure)	Yes (at vessel failure)
IRWST cavity injection	No	No	No
Main Feedwater	No	No	No
Startup Feedwater	No	No	No
PCS sprays	Yes	Yes	Yes
PRHR system	No	No	No
Discharge Compartments	SG1 and IRWST	SG1	IRWST (+ a small steam flow in the U.C. Dome)
H_2 produced (kg)	630	689	710

3. Application of HOCRA to accidents in an advanced PWR

There are many severe accident sequences in which the hydrogen mitigation system may have to intervene. For an advanced PWR, Westinghouse selected three reference scenarios, named HYD1, HYD2 and HYD3, from the most probable accident sequences, according to the probabilistic risk analysis (PRA), to show that the deliberate ignition system they chose meets the requirements of 10 CFR 50.34(f) [11].

In a LOCA, the release of steam and hydrogen in the containment takes place in the compartment where the primary system failure is located and/or in the compartment where the automatic depressurization system (ADS) is discharging. The quantity of steam and H_2 released will be diluted in the free volume of the containment in proportion to the discharge velocity and buoyancy.

Table 1 summarizes the situation of the reactor in the three cases. It presents the initial cause and the operating conditions of the intervention systems that determine the accident evolution, along with the compartments where the discharge takes place and the overall mass of hydrogen produced, estimated by Westinghouse with the MAAP 4.0 computer code.

The zirconium present in the active core is estimated to be 14 380 kg. The metal-water reaction produces two hydrogen moles for each mole of oxidized zirconium. In accordance with the requirements specified in 10 CFR 50.34(f) (100% oxidation), all the accident scenarios are assumed to generate a quantity of hydrogen equal to at least

635.6 kg. In the MAAP 4.0 calculations in which the overall mass of hydrogen produced would have been less than the quantity required, the input data were artificially modified in order to force the code to increase the production of hydrogen. The contact surface Zr-H_2O and the parameter that controls the collapse of the core were varied at the same time so as to alter them the least possible, the only aim being to go over 635.6 kg.

The simulations with MAAP 4.0 of the three scenarios show that the hydrogen fraction in the containment increases rapidly once the discharge has begun (2-4 hours after the beginning of the accident). They also highlight that the molar fractions of the gases in the various compartments are very similar to each other except for in the IRWST in cases HYD1 and HYD3. In all cases, the pressure is uniform between the various compartments. The thermodynamic conditions in the containment are therefore able to promote a degree of mixing of the atmosphere which is sufficient to homogenize the hydrogen (and the steam) in most of the free volume, apart from in the IRWST, when the discharge takes place there.

The definition of a system of catalytic recombiners for the examined advanced PWR can then be developed in two stages:

1) Evaluate the feasibility and capability of a recombiner system to control the hydrogen in accordance with the requirements outlined in 10 CFR 50.34(f) in the whole containment apart from the IRWST. Since the free volume of the IRWST gives a small contribution (~ 1%) to the overall free volume (~ 48 650 m^3) and the molar fraction of hydrogen in it is greater or equal to the average in the containment, it is reasonable to assume that this system of recombiners is conservatively sized by applying HOCRA mode-1 to the whole volume of the containment.
2) Identify a mitigation system that is suitable for controlling the hydrogen in the IRWST volume, with a local analysis carried out with HOCRA mode-2.

3.1 Calculations with HOCRA mode-1

HOCRA mode-1 has been applied, both for NIS and 'large' Siemens recombiners, at the releases of hydrogen foreseen in the accident scenarios HYD1, HYD2 and HYD3.

Figures 4-6 show the variations in time of the discharge rate, W_{H2}, the overall recombination rate for the system of NIS or Siemens recombiners, R_{rN} or R_{rS}, and the "dry" volumetric concentration (i.e. evaluated only taking into account hydrogen and air) without, Cd_{0H2}, and with the NIS or Siemens recombiners, Cd_{NH2} or Cd_{SH2}.

In addition, for an analysis of the sensitivity of the code to the release typology, HOCRA mode-1 was also applied to the transient assumed by EPRI for evaluating the capability of a NIS recombiner system [5] (Fig. 7):

- 50% of the release in the first 10 min after the beginning of the accident
- 25% of the release in the following 35 min
- 25% in the following 50 min

All the elaborations were made assuming that:

V = 48 652 m^3, free volume of the containment
P_{0a} = 101 325 Pa, partial pressure of the air at T_0 = 298.15 K

The air amount in a containment is practically invariable before venting, therefore the "dry" H_2 volumetric concentration only depends on the H_2 molar density.

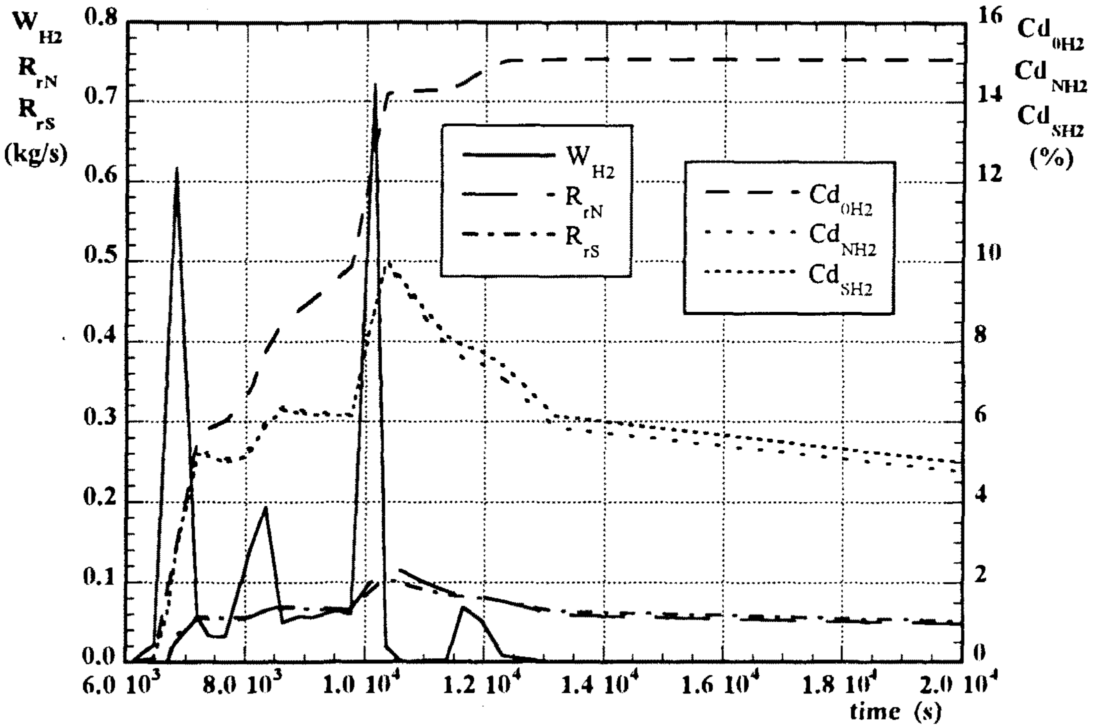

Figure 4. HYD1 scenario

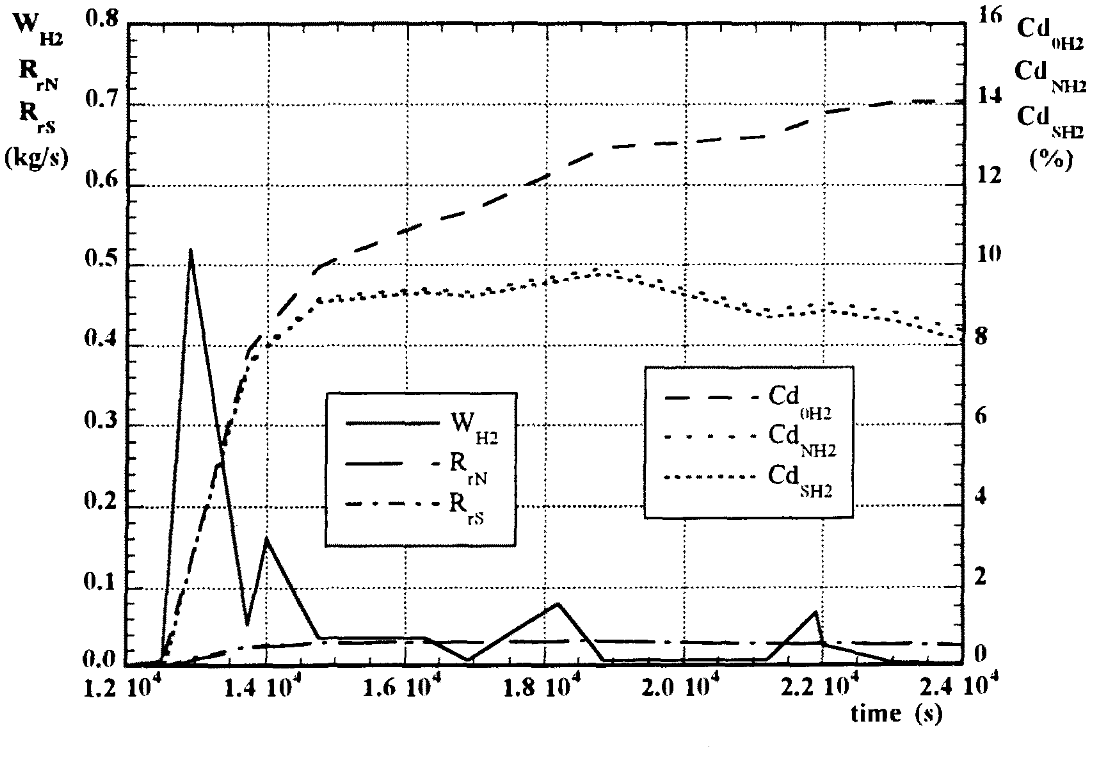

Figure 5. HYD2 scenario

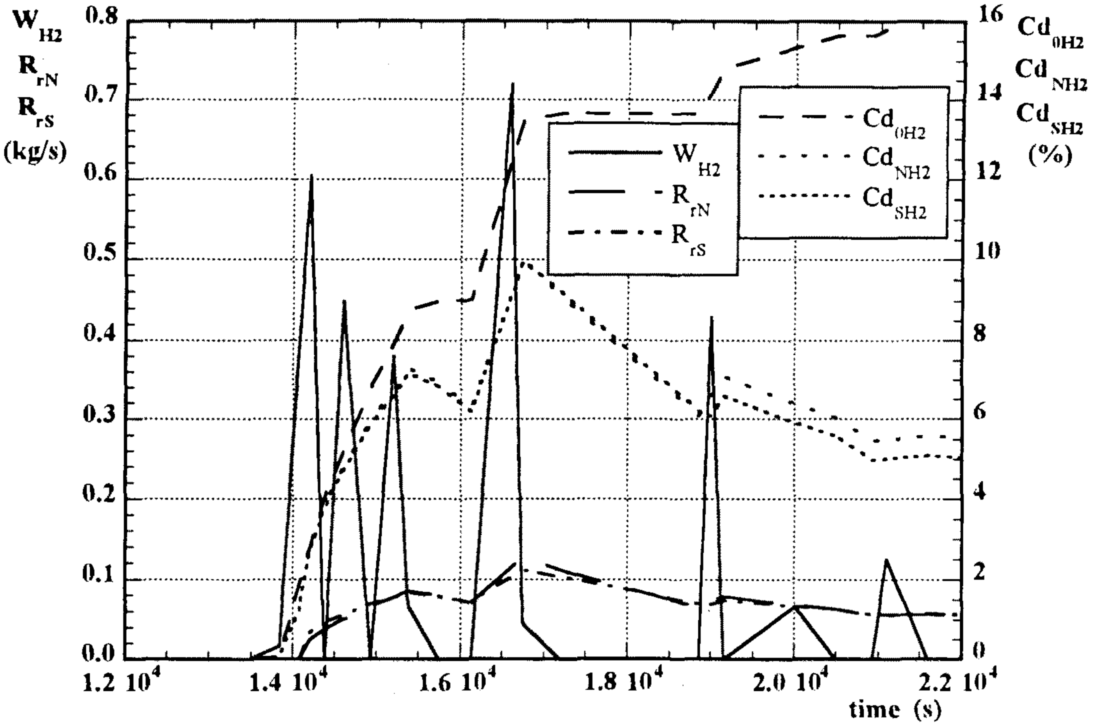

Figure 6. HYD3 scenario

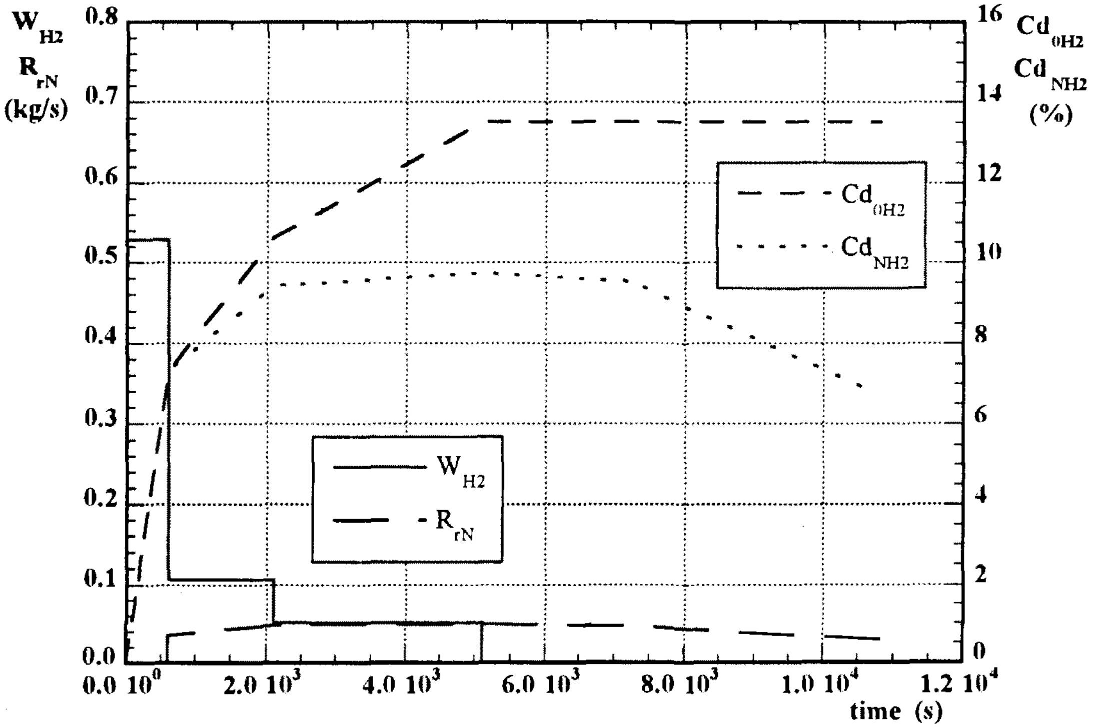

Figure 7. EPRI scenario

Table 2. Results of the analysis made with HOCRA mode-1 of the three accident scenarios

Accident	H_2 released (kg)	NIS			Siemens "large"		
		Rec. No	Cd_{H2} max	Cd_{H2} (12h)	Rec. No	Cd_{H2} max	Cd_{H2} (12h)
HYD1	712.0	47	9.97 %	0.04 %	39	10.00 %	0.00 %
HYD2	660.5	12	9.92 %	1.54 %	12	9.78 %	0.53 %
HYD3	785.0	48	9.98 %	0.02 %	42	9.98 %	0.00 %

For both types of recombiner a start-up time of 600 s was imposed and fixed in all the executions. During this time it was assumed that the recombiner was not functioning, so as to simulate the response of a roughly first-order system with the response of a zero-order system with dead time.

The data on the release rate were derived from the graphics supplied for the various accident scenarios calculated with MAAP 4.0 [11]. In this operation a sufficient number of data was sampled to reproduce the release typology and to obtain an overall mass of hydrogen that was greater than the minimum indicated in accordance with 10 CFR 50.34.

HOCRA searches for the minimum number of recombiners needed to maintain the "dry" volumetric hydrogen concentration below a given limit throughout the whole transient. Limiting the "dry" volumetric hydrogen concentration is important because the maximum theoretical static overpressure due to a deflagration is proportional to the H_2 molar density. In addition, the likelihood of detonation in a hypostoichiometric mixture increases with the H_2 volumetric concentration, which is conservatively estimated with the "dry" value because this is independent of steam and thus the containment temperature. The chosen limit was 10% in accordance with 10 CFR 50.34 f.2.ix.

Table 2 summarizes, for each type of accident and recombiner, the total mass of hydrogen calculated by the code, the number of recombiners determined on the basis of the criterion mentioned above, the maximum volumetric concentration of hydrogen and the one after 12 h from the beginning of the release.

The results confirm that the number of recombiners calculated is essentially a consequence not so much of the total mass to "burn" but of the release rate when Cd_{H2} is near to the limit value imposed. A strong initial discharge of hydrogen (when the concentration is still below the limit imposed for the sizing), which is followed by a modest release rate, such as in HYD2, requires a lower number of recombiners than a hydrogen release that evolves in an inverse manner, as in HYD1 and HYD3.

The transient assumed by EPRI, Fig. 7, is very close to case HYD2: in the simulation with the NIS recombiner system, the code finds that 19 recombiners are needed to maintain $Cd_{H2} < 10\%$ in vol., which is in very good agreement with the 20 indicated in [5].

3.2 Calculations with HOCRA mode-2

HOCRA mode-2 was applied to the SG1, SG2 and IRWST compartments in the HYD1 accident scenarios.

The input data of HOCRA mode-2, concerning the transients of pressure, temperature, and molar fractions of hydrogen and steam for the various compartments, were derived from the graphics produced by the calculations made with MAAP 4.0 without recombiners [11].

Two executions were carried out for each compartment examined, in one the NIS recombiner was used, in the other the 'large' Siemens recombiner. The hydrogen transients calculated by the code do not show much difference between the two series of cases. Furthermore, the results for the SG1 and SG2 compartments are similar since there is a considerable affinity of accident evolution in the two volumes.

For the SG1 (free volume ~ 1160 m^3) and SG2 (free volume ~ 950 m^3) compartments, the results of HOCRA mode-2 show that only one recombiner for each volume would be able to maintain the "dry" volumetric concentration of hydrogen lower than 10%, with a peak value of around 9%. Leaving aside the structural differences of HOCRA modes -1 and -2 which make questionable any comparison of the results obtained from the two calculations, this result is in agreement with what was determined with HOCRA mode-1, that is 1 recombiner for about every 1000 m^3 (1 in 1000 m^3 for the NIS model, 1 in 1250 m^3 for the large Siemens).

The analysis of the SG1 and SG2 compartments carried out with HOCRA mode-2 should rather be utilized for a comparison with what was obtained with the HOCRA mode-2 for IRWST.

In IRWST, the "dry" volumetric concentration of hydrogen increases suddenly even in the first instants following the beginning of the H_2 release and reaches values of around 20% before the recombiners come into action after the start-up time. Obviously, in these conditions no recombination system is able to maintain $Cd_{H2} < 10\%$ for all the transient. The release rate peaks (both the initial one described above, and the later ones) are so high that, even if a null start-up time is assumed, the code cannot determine a realistic number of recombiners that can control the rise in concentration.

The analysis conducted with two recombiners in the IRWST shows that the concentration of hydrogen is maintained practically at zero for all the time outside the release peak intervals, during which the system is actually not able to counter the increase in "dry" concentration which goes above 10%.

Although the conservativeness of "dry" evaluations should be taken into account, the comparison with the results obtained for the SG1 and SG2 compartments highlights the difficulties that the system of recombiners would have in controlling the hydrogen concentration in the IRWST in some accidents.

4. Conclusions

The optimum number and location of catalytic recombiners in a nuclear reactor containment that are needed to cope with the hydrogen generated during an accident, depend on the H_2 release rate (either in relation to the accident being examined or assumed by possible safety rules) and on the prediction of distribution of the gas mixture chemical composition by computer codes much more than it is for a system of ignitors. The capacity to predict H_2 generation and distribution is increasing, but there will inevitably be some limits to the level of detail. Uncertainties will always be linked to the degree to which the data obtained in scale model containments can be applied to full size reactor containments.

If recombining is the only mitigation measure for hydrogen, the number of recombiners to be installed in a nuclear reactor containment has to balance the H_2 release rate when the "dry" H_2 concentration reaches the maximum "acceptable" value. The number of recombiners calculated could be very different if this balance has to be satisfied in the whole containment or even locally, in every compartment. In this last case, a feasible number of recombiners could be used, if ignitors are provided in the most critical compartments. This number could be increased, to take into account any uncertainty in predicting H_2 generation and mixing as well as recombiner capacity. Additional mitigation measures, such as deliberate ignition or post-dilution, for scenarios with high hydrogen release rates, might be indispensable for controlling hydrogen.

Specifically, some first attempt calculations were carried out to verify the possibility of using a system of passive recombiners to control the hydrogen in an advanced PWR. The results were encouraging, though also ignitors seem to be needed to control the hydrogen in the IRWST.

Research will be needed to define better in theoretical and semi-empirical terms the behavior and the effects of the passive catalytic recombiners located in large volumes in post-accident thermal-hydraulic conditions. In addition, the containment codes will have to be directly implemented with recombiner models in order to better ascertain the number and location of the recombiners.

The regulatory requirements about hydrogen in severe accidents should be reviewed as well, to adapt them to new mitigation measures. In fact, at present, safety rules provide the maximum amount of H_2 that can be generated (e.g. equal to the H_2 generated by the oxidation of 100% of the total zirconium inventory, according to 10 CFR 50.34 f.2.ix) and the maximum acceptable H_2 molar density (e.g. $Cd_{H2} = 10\%$, according to 10 CFR 50.34 f.2.ix). This may be enough to design pre-inerting and deliberate ignition systems, but the most important parameter to determine the number and location of the catalytic recombiners or injection nozzles of a H_2 dilution system is *the H_2 generation rate, which, for example, 10 CFR 50.44 c.1+d.1+d.2 only provides* for the Design Basis Accidents in connection to the use of the old types of active recombiners (a time period of 2 minutes is the interval after a postulated LOCA over which the oxidation of 5% of the total zirconium inventory should occur).

Nomenclature

ADS: Automatic Depressurization System
Cd = "dry" volumetric concentration
IRWST: In-containment Refueling Water Storage Tank
J = molar flow rate (mol/s)
LOCA: Loss Of Coolant Accident
M = molecular weight (kg/mol)
n = mole number
N = recombiner number
NVI = compartment number
P = pressure (Pa)
PCS: Passive containment Cooling System
PRHR: Passive Residual Heat Removal system
PWR: Pressurized Water Reactor
R = Correlation Coefficient
R_r = recombination rate, that is the hydrogen mass recombined in the unit of time by a recombiner (kg/h or kg/s)
SG1/2: compartments where a steam generator is located
t = time (s)
T = temperature (K)
U.C.: Upper Containment compartments
V = volume (m^3)
W = discharge rate (kg/s)
[X] = concentration, or molar density, of the chemical species X (mol/m^3)
Φ = fuel equivalence ratio $= \dfrac{n_{H_2}/n_{O_2}}{\left(n_{H_2}/n_{O_2}\right)_{stoich}} = \dfrac{1}{2}\,\dfrac{[H_2]}{0.21\,[air]_0}$;
when the molar density of the air is invariable (in Fig. 3 it is equal to the STP gas molar density, $[air]_0 = 44.64\ mol/m^3$), Φ only depends on the hydrogen molar density.

Indices

0 = initial conditions or without recombiners
a = air
i = inlet
N = related to the NIS recombiners
o = outlet
H_2 = related to hydrogen
O_2 = related to oxygen
r = related to a recombiner
stoich: stoichiometric
S = related to the Siemens large recombiners
t = total (conditions refer to all the containment)

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