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COGAP: A Nuclear Power Plant Containment Hydrogen Control System Evaluation Code

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Prepared for
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Commission

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COGAP: A NUCLEAR POWER PLANT CONTAINMENT HYDROGEN
CONTROL SYSTEM EVALUATION CODE

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ABSTRACT

The accounting of containment gas concentration following a loss-of-coolant accident is important in the safety evaluation of hydrogen combustible-gas control systems for nuclear power plants. The COGAP code provides such accounting including the effects of (1) the reaction of zirconium and water; (2) radiolysis of core and sump water; (3) corrosion of zinc, aluminum and copper; (4) recirculation between compartments; (5) hydrogen recombiners; (6) purging; (7) nitrogen addition; and (8) atmospheric steam. Controls are available to determine when options are initiated; for example, the hydrogen recombiner can be started when the hydrogen concentration reaches a user-specified value.

I. INTRODUCTION

Following a loss-of-coolant accident (LOCA), hydrogen gas may accumulate within the containment of a nuclear power plant. The hydrogen could result from (1) metal-water reaction involving the zirconium fuel cladding and the reactor coolant; (2) radiolytic decomposition of water, which will produce oxygen also; and (3) corrosion of construction materials. A potentially hazardous situation could result if there is sufficient oxygen to promote hydrogen burning or detonation. Therefore, calculations must be performed to determine the gas concentrations in the containment and the effect of combustible-gas control systems, that might be used to keep the gas concentrations at acceptable levels, such as recombiners.^{1,2} The COGAP

(Combustible Gas Analysis Program) code was written to perform such calculations.

COGAP was written by D. Shum of the Nuclear Regulatory Commission (NRC) where it was referred to as COGAP-II (Ref. 3). COGAP-II was written as a replacement for the original COGAP (Ref. 4) used by the NRC for many years to evaluate containment combustible-gas control systems for nuclear power plants. COGAP-II was sent to Los Alamos for review, modification, and public release through the National Energy Software Center in Argonne, Illinois. For convenience, the original name COGAP was retained.

II. DISCUSSION

In this section the various features of COGAP are discussed. Additional insight into the code may be obtained from the Description of Input in Appendix A and the Sample Problems in Appendix B. The discussion that follows will be presented in terms of sources of hydrogen (and sometimes oxygen) and means of controlling the gas concentrations.

A. Hydrogen Sources

1. Oxidation of Core Zirconium. Hydrogen can be generated during a LOCA by the reaction of hot zirconium cladding with the surrounding steam. The equation used for this reaction in COGAP is



The amount of hydrogen generated is controlled by user specification of the total core zirconium and the per cent of the total that is oxidized. The hydrogen generated is added to compartment number one only as a linear function of time over a user-specified interval after the end of blowdown.

2. Radiolysis of Core and Sump Water. Following a LOCA, hydrogen and oxygen can be produced in the core and sump by radiolysis of water according to the equation



The core cooling water radiolysis primarily results from gamma radiation energy produced by the decay of fission fragments in the fuel. The sump water radiolysis results from the energy produced by the decay of fission fragments and heavy elements dissolved in the sump water. The rate of hydrogen and oxygen production due to radiolysis therefore is dependent on the (1) energy production rate as a function of time, (2) fraction of the energy that is absorbed by the water, and (3) the hydrogen yield per unit of energy absorbed (the oxygen yield will be 0.5 of the hydrogen yield). The general format for the calculation of hydrogen production due to radiolysis is described below. The energy production rates, which are based primarily on Ref. 5, are described in greater detail in Appendix C. Reference 6 provides guidance regarding the values of the user-specified parameters that affect the radiolytic hydrogen production. Note that the hydrogen and oxygen due to radiolysis of the core water are deposited initially into compartment one. The hydrogen and oxygen due to radiolysis of the sump water are distributed according to the user-input compartment FRC parameter.

In equation form, the total hydrogen production can be expressed by (see Ref. 2, Sect. 6.2.5, Appendix A)

$$S_H = \frac{P}{B N} \frac{G_C E_C + G_S E_S}{100} \quad , \quad (3)$$

where

S_H = hydrogen production rate, H_2 lb_m-mole/s;

P = reactor operating thermal power level, MW_t, a user-specified value;

B = conversion factor, 454 g-mole/lb_m-mole;

N = Avagadro's number, 6.023×10^{23} H_2 molecules/g-mole;

G_C = radiolytic hydrogen yield [$G(H)_C$] in the core water relative to the energy absorbed, H_2 molecules/100eV, a user-specified value;

E_C = fission product gamma decay energy absorbed by the core water, eV/(s-MW_t), see Eq. (4) below;

G_s = radiolytic hydrogen yield $[G(H)_g]$ in the sump water solution relative to the energy absorbed, H_2 molecules/100eV, a user input value; and

E_s = dissolved radioisotope decay energy absorbed by the sump water, $eV/(s-MW_t)$, see Eq. (5) below.

The expression $G(H)$ is introduced because of its use in Ref. 6 and Appendix A, COGAP Input Description. The E_c term in Eq. (3) is defined by

$$E_c = (f_\gamma)_c H_\gamma \quad , \quad (4)$$

where

$(f_\gamma)_c$ = fraction of total gamma decay energy absorbed by the core water, a user input value, and

H_γ = total fission product gamma decay energy production rate, $eV/(s-MW_t)$, see Appendix C.

The E_s term in Eq. (3) above is defined by

$$E_s = (f_{\gamma+\beta})_s H_{\gamma+\beta} + (f_I)_s H_I \quad , \quad (5)$$

where

$(f_{\gamma+\beta})_s$ = fraction of total dissolved-solid decay energy absorbed in the sump water outside the core;

$H_{\gamma+\beta}$ = total dissolved-solid decay energy production rate, $eV/(s-MW_t)$, see Appendix C;

f_I = fraction of radioiodine decay energy absorbed in the sump water outside the core; and

H_I = radioiodine decay energy production rate, $eV/(s-MW_t)$, see Appendix C.

3. Reaction of Containment Surfaces. Another possible source of hydrogen could be from metal surfaces exposed to environments containing high-temperature steam, corrosive sprays, fission products, and radioactivity. Such exposure might result in surface corrosion reactions that produce hydrogen. Surfaces composed of aluminum, zinc (including galvanized and

zinc-base painted surfaces), and copper are candidates. Corrosion tests have been performed to determine the behavior of the various metals used in the containment when exposed to emergency core cooling solutions at reference design-base-accident conditions.

The chemical equations used in COGAP to determine the hydrogen generated due to corrosion are



Thus, 1.5, 1.0, and 1.0 moles of hydrogen are generated for each mole reacted of aluminum, zinc, and copper, respectively. The hydrogen production rates are completely controlled by user input of corrosion surface area, surface thickness, and rate of corrosion.

4. Hydrogen (and Oxygen) Dissolved in Primary Coolant. The moles of hydrogen and oxygen dissolved in the primary coolant during normal operation can be specified by input. These are released in the first time step of the COGAP calculation. Distribution of these gases is controlled by the compartment FRC parameter, which is specified for each compartment by the user. Each compartment's fractional distribution is based on the compartment FRC fraction of the sum of the FRC for all compartments, which is described in the Appendix A input description.

B. Gas Concentration Control Options

Gas concentrations and their control are based on the ideal gas equation

$$P V = N R T \quad ,\tag{7}$$

where P is the absolute pressure, V is the volume, N is the total number of gas moles, R is the universal gas constant, and T is the absolute temperature.

As a result, constant volume flow rate fans (that is, constant rotations per unit time) transfer gas moles according to

$$\frac{dN}{dt} = \frac{dV}{dt} \times \frac{P}{R \times T} , \quad (8)$$

where t is time and P and T are the pressure and temperature for the flow source. These equations are used to exercise the control options that are described in the following.

Note that all flow devices in COGAP are assumed to have a constant volumetric flow rate specified by the user in cubic feet per minute (cfm). The resulting molar flow rate is that based on Eq. (8) with the pressure and temperature being those for the flow source. If the flow source is a compartment, its pressure and temperature are used with (a) temperature specified by the initial-temperature and the temperature-variation-with-time inputs and (b) pressure calculated from Eq. (7). The nitrogen addition and purging flow sources are assumed to be at standard ambient conditions of 14.7 psia and 70 °F. Ambient flow sources at different conditions can be specified by modification of the cfm on the basis of Eq. (8). For example, an ambient flow source at a pressure of 2×14.7 psia would require a cfm specification that is twice that for the same volumetric flow rate of an ambient flow source at 14.7 psia.

1. Steam Accounting. To include the presence of steam and its effect on gas concentrations, an input flag must be set. This allows use of the initial compartment relative humidity to specify the initial amount of steam in each compartment; this in turn is based on relative humidity as the ratio of the steam partial pressure to the steam saturation pressure at the compartment initial temperature. The steam partial pressure then is used in Eq. (7) to determine the compartment steam moles. For each time thereafter, the number of steam moles in each compartment is determined from an input table of temperatures vs time. These temperatures are taken to be the steam saturation temperatures in the compartments from which corresponding steam partial pressures are obtained. The compartment steam moles then are determined from Eq. (7). Note that this procedure results in compartment steam mole content

that is independent of mole transfer functions such as recirculation and purging. However, the presence of steam on the concentrations of other gases is accounted for in the transfer calculations. The steam option is not part of the accepted method of licensing analysis and is provided only for the convenience of the user.

2. Purging. A purge for each compartment can be specified. The purge causes the addition of air at standard ambient conditions to the compartment and the removal of compartment contents at the compartment conditions that existed at the beginning of the time step. The addition and removal are calculated by Eq. (8) for the user-specified volumetric flow rate. The purge could cause the compartment gas concentrations to change because the mixtures being exchanged could have different concentrations. In addition, the total gas moles in the compartment could change because the mixtures being exchanged could have different densities.

3. Nitrogen Addition. Nitrogen addition is specified by giving a nonzero value for the volumetric flow rate of the addition. The nitrogen is assumed to be at standard ambient conditions with the moles added determined by Eq. (8). The addition is made for all times. Note that the addition of nitrogen from a source with values of pressure and temperature different from standard conditions could be accomplished by modification of the volumetric flow rate based on Eq. (8).

4. Recirculation. The exchange of compartment contents can be specified by identification of the (1) number of recirculation connections, (2) compartments involved in each connections, and (3) volumetric flow rates for each connection.

5. Hydrogen Recombiners. Several recombining connections can be specified to modify the hydrogen and oxygen concentrations of the compartments at specified volumetric flow rates. The recombined flow can be designated to (1) return to the source compartment, (2) be returned to any other compartment, or (3) not be returned to any compartment. Recombiners can be specified to begin on the basis of (1) an initiation time, (2) the hydrogen concentration in a particular compartment, or (3) the average hydrogen concentration for all compartments.

REFERENCES

1. "Control of Combustible Gas Concentrations in Containment Following a Loss-of-Coolant Accident," Regulatory Guide 1,7, Revision 2, U. S. Nuclear Regulatory Commission (November 1978).
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3. D. H. Shum, "Development of a Code (COGAP-II) for Evaluation of Combustible Gas Concentrations and Mixing in Various Compartments of a Containment," Memo to Z. R. Rosztoczy, Chief, Analysis Branch, Division of Systems Safety, U. S. Nuclear Regulatory Commission (September 16, 1976).
4. J. A. Kudrick, "Computer Program (COGAP) for Predicting Containment Hydrogen and Oxygen Concentrations Following Loss-of-Coolant Accidents," Memo to R. L. Tedesco, Assistant Director for Containment Safety, Atomic Energy Commission, Directorate of Licensing (December 2, 1972).
5. "Residual Decay Energy for Light Water Reactors for Long-Term Cooling," Branch Technical Position APCSB 9-2, attached to Section 9.2.5 of Ref 2.
6. "Control of Combustible Gas Concentrations Following a Loss-of-Coolant Accident," Branch Technical Position CSB 6-2, attached to Section 6.2.5 of Ref. 2.

APPENDIX A

COGAP INPUT DESCRIPTION

This appendix presents the COGAP input format, variable names, dimensional units, and variable descriptions. Note that necessary cards are identified by use of the word REQUIRED in upper case letters. Reference to a card is made by using the referenced card name with the first letter of each card description word in upper case, for example, the note for the Integer control parameters card refers to the Temperature vs Time Sets card. Volumetric flow rates are specified in cfm with the molar flow rates based on the flow source pressure and temperature by Eq. (8). The purge and nitrogen addition flow sources are assumed to be at the standard conditions of 14.7 psia and 70°F. The expression NE means not equal.

TITLE CARD(18A4) - one card REQUIRED

INTEGER CONTROL PARAMETERS (7I5) - one card REQUIRED

Word/Last Column	VARIABLE Units	Description
1/5	ICON(1) none	Specifies use of purge and recombiner where 1 = No purge and no recombiner; 2 = With purge only; 3 = With recombiner only.
2/10	ICON(2) none	Specifies whether there are more cases where 0 = Last or only case; NE 0 = Another set of input follows.
3/15	ICON(3) none	Plot control, which currently is unavailable, where 0 = No plots; NE 0 = With plots.
4/20	ICON(4) none	Number of compartments (1 min, 5 max).
5/25	ICON(5) none	Number of connections between compartments for recirculation (20 max).

- 6/30 ICON(6) Specifies H₂ concentration for comparison with CON(3)
none (Floating Point Control Parameters card) to decide
when purging or recombination should be initiated.
0 = Average of all compartments used;
X = Concentration of compartment X used.
- 7/35 ICON(7) Specifies accounting of steam where
none 0 = No steam accounting;
NE 0 = With steam.

Note - Initial steam content for individual compartments is based on the Compartment Specifications card variable RELHUM(i). At later times, compartment steam content is based on its atmosphere being saturated at the temperature specified in the Temperature vs Time Sets card below, see Sec. II.B.1.

FLOATING POINT CONTROL PARAMETERS (5F10.0) - one card REQUIRED

Word/Last Column	VARIABLE Units	Description
1/10	CON(1) days	Problem end time.
2/20	CON(2) days	Purge or recombiner initiation time.
3/30	CON(3) %	H ₂ concentration at which purging or recombination begins. CON(2) must be zero to use this option.
4/40	CON(4) days	Recirculation fan(s) start time.
5/50	CON(5) s	Interval after end of blowdown over which H ₂ from the Zr-H ₂ O reaction is linearly released into compartment one.

COMPARTMENT SPECIFICATION (8F9.0) - ICON(4) cards expected

Compartments will be numbered in the order of entering these cards. The i index is the compartment number. Note that the first compartment is special because of the hydrogen release due to the Zr-H₂O reaction and the H₂ and O₂ due to radiolysis of the core water enter only compartment one.

Word/Last Column	VARIABLE Units	Description
1/9	V(i) ft ³	Compartment volume.
2/18	PA(i) lb _f /in ²	Total pressure.

3/27	PN(i) lb _f /in ²	Nitrogen partial pressure. If the total pressure is equal to PN(i) and there is steam, the nitrogen partial pressure is reduced to accommodate the steam. A PN(i) of zero results in the nitrogen and oxygen mole fractions of air.
4/36	T(i) °F	Initial temperature. If there is steam indicated, this temperature will be the initial saturation temperature, see RELHUM(i) that follows.
5/45	RELHUM(i) none	Initial relative humidity, which is PV(i)/PSAT, where PV(i) is the steam partial pressure and PSAT is the steam saturation pressure at T(i).
6/54	HP(i) cfm	Purge volumetric flow rate of ambient air added to this compartment with an equal volumetric flow rate removed from this compartment.
7/63	FRC(i) %	Factor used to determine the distribution of the hydrogen and oxygen (a) dissolved in the reactor coolant water and (b) generated by radiolysis of sump water. The moles added to each compartment are the product of the total moles available and the FRC(i) divided by 100. Thus, the FRC(i) can be interpreted as a percentage if they sum to 100.
8/72	ADN(i) cfm	Nitrogen addition rate.

CONNECTION SPECIFICATION (2I5, F10.0) - ICON (5) cards expected
j is a connection index based on the order of inputting these cards

Word/Last Column	VARIABLE Units	Description
1/5	NJ1(j) none	Compartment at connection inlet. A zero value will result in nothing happening to compartment NJ2(j).
2/10	NJ2(j) none	Compartment at connection outlet. A zero value will result only in removal from the NJ1(j) compartment.
3/20	VR(j) cfm	Volumetric flow rate between compartments.

FIRST REACTOR COOLANT PARAMETER CARD (6F10.0) - one card REQUIRED

Word/Last Column	VARIABLE Units	Description
1/10	RC(1) MW _t	Reactor thermal power.
2/20	RC(2) h	Reactor operating time.
2/30	RC(3) lb _m	Zirconium mass.
4/40	RC(4) %	Per cent zirconium reacted with water. The resulting hydrogen is added to compartment one only.
5/50	RC(5) lb _m -mole	Oxygen dissolved in reactor coolant water.
6/60	RC(6) lb _m -mole	Hydrogen dissolved in reactor coolant water.

Note - The dissolved oxygen and hydrogen are added to each compartment over the first time step according to $FRC(i) \times RC(5) / 100$ and $FRC(i) \times RC(6) / 100$, respectively, with $FRC(i)$ from the Compartment Specification card.

SECOND REACTOR COOLANT PARAMETER CARD (6F10.0) - one card REQUIRED

Word/Last Column	VARIABLE Units	Description
1/10	RC(7) molecules /100 eV	Radiolytic hydrogen yield $G(H)_c$ in core water used in Eq. (3). This hydrogen and the associated oxygen go to compartment one only.
2/20	RC(8) molecules /100 eV	Radiolytic hydrogen yield $G(H)_s$ in sump water solution used in Eq. (3).
3/30	RC(9) per cent	Per cent fission-product decay energy absorbed by the core water, resulting in radiolysis and the generation of hydrogen and oxygen, which are added to compartment one.
4/40	RC(10) per cent	Per cent of total solid fission-product decay energy absorbed by the sump water solution.

5/50 RC(11) Per cent of total iodine isotope decay energy
per cent absorbed by the sump water solution.

6/60 RC(12) Reactor coolant blowdown time used to determine
s the time after which the Zr-H₂O reaction hydrogen
is introduced into compartment one.

Note - RC(8), RC(10) and RC(11) affect the hydrogen and oxygen generation due to sump water radiolysis.

NUMBER OF CORROSION SURFACES (I5) - one card REQUIRED

Word/Last Column	VARIABLE Units	Description
1/5	NC none	Number of aluminum, zinc, or copper corrosion surfaces (10 max).

CORROSION SURFACE DESCRIPTION (2I5, 2F10.0) - NC cards expected
i is surface number index based on the order of entering these cards

Word/Last Column	VARIABLE Units	Description
1/5	IVO(i) none	Number of compartment in which surface is located.
2/10	MAT(i) none	Identification of surface material where 1 = aluminum, 2 = zinc, 3 = copper.
3/20	SURF(i) ft ²	Surface area.
4/30	THK(i) in.	Surface thickness.

NUMBER OF TIMES FOR CORROSION RATE SPECIFICATION (4F10.0) - one card expected
if NC (Number of Corrosion Surfaces card) is not zero

Word/Last Column	VARIABLE Units	Description
1/5	NPT none	Number of cards that follow for specification of corrosion rate vs time (2 min, 10 max).

CORROSION RATES VS TIME (4F10.0) - NPT cards expected (only if NC ≠ 0)

The values of time must be increasing. i is the order of reading the cards.

Word/Last Column	VARIABLE Units	Description
1/10	TIMEV(i) days	Time.
2/20	ACOR(i) mil/yr	Aluminum corrosion rate at time TIMEV(i).
3/30	ZCOR(i) mil/yr	Zinc corrosion rate at time TIMEV(i).
4/40	CCOR(i) mil/yr	Copper corrosion rate at time TIMEV(i).

Note - More sets can be provided in a similar manner on additional cards.

NUMBER OF TIME INTERVALS AND DIAGNOSTIC CONTROL (I5, 2F10.0) - one card REQUIRED

Word/Last Column	VARIABLE Units	Description
1/5	KTIME none	Number of intervals that can have different time steps and print intervals (1 min, 20 max).
2/15	TIDIINI days	Time at which diagnostic printing begins.
3/25	TIDIFIN days	Time at which diagnostic printing ends.

TIME STEP AND PRINT CONTROL (2F10.0, 2I10) - KTIME cards expected
i is the order of reading the cards.

Word/Last Column	VARIABLE Units	Description
1/10	TIMEX(i) days	Time at beginning of interval.
2/20	TIMEY(i) days	Time increment used for performing calculations within interval.

3/30 NPRINT(i) Number of time steps between prints.
 none

4/40 NPLOT(i) Number of time steps between points plotted; however,
 none plotting is currently unavailable.

Notes - To get printed output at TIMEX(i+1), the NPRINT(i) and TIMEY(i) should be specified to produce output at TIMEX(i+1).

Also, the time increments [TIMEY(i)] (1) must be sufficiently small to preclude the removal of more moles from a volume than are available, (2) should be varied to establish that the results of interest are not affected by the time increment size, and (3) are required to satisfy (1) when the steam option is used has been found to be smaller than when this option is not used; e. g., the Appendix B sample problem time increments had to be reduced by a factor of 10 when the steam option was included.

NUMBER OF TEMPERATURE VS TIME SETS (15) - one card REQUIRED

Word/Last Column	VARIABLE Units	Description
1/5	NT1 none	Number of time-temperature sets (2 min, 20 max).

Note - The temperatures that follow will be the those for all compartments after zero time. The zero time temperature is specified on the Compartment Specification card. If ICON(7) of the Integer Control Parameter is zero, these temperatures only result in a change in the compartment pressures by Eq. (7). The accounting of steam may be called for by ICON(7) of the Integer Control Parameter card as nonzero. In this case, these temperatures are the compartment steam saturation temperatures for the determination of compartment steam moles.

TIME VS TEMPERATURE SETS (6F10.0) - cards expected based on NT1 and the fact that three sets can be specified per card

Word/Last Column	VARIABLE Units	Description
1/10	TME(1) days	First set time.
2/20	TEMP(1) of	First set temperature.

3/30	TME(2) days	Second set time.
4/40	TEMP(2) °F	Second set temperature.
5/50	TME(3) days	Third set time.
6/60	TEMP(3) °F	Third set temperature.

Note - More sets can be provided in a similar manner on additional cards.

NUMBER OF HYDROGEN RECOMBINER CONNECTIONS (I5) - one card expected only if ICON(1) on the Integer Control Parameter card is three

Word/Last Column	VARIABLE Units	Description
1/5	NT3 none	Number of hydrogen recombiner connections (20 max).

HYDROGEN RECOMBINER CONNECTIONS (2I5, F10.0) - NT3 cards expected
j is the order of reading these cards.

Word/Last Column	VARIABLE Units	Description
1/5	NR1(j) none	Compartment that provides flow to a recombiner. NR1(j) = 0 results in no flow into compartment NR2(j) due to this connection.
2/10	NR2(j) none	Compartment that receives flow from NR1(j) after recombination. NR2(j) = 0 results in flow removal from NR1(j) only; and NR2(j) = NR1(j) results in the recombined flow being returned to NR1(j).
3/20	HR(j) cfm	Recombiner volumetric flow rate.

Note - More connections can be specified in a similar manner on additional cards.

APPENDIX B

SAMPLE PROBLEMS

Figure B-1 presents the output for two sample problems, which were constructed to demonstrate the various code options and therefore may not be representative of "real" problems. Note that the output includes a listing of the input cards, interpretive descriptions of the input, and the calculated results. The sample problems are described briefly below even though they could be constructed from the input.

Sample Problem 1

The integer-control parameters specify that there will be purging, an additional case (Sample Problem 2), no plotting, one compartment, no recirculation connections, purge initiated when the compartment one hydrogen concentration exceeds a specified value, and there is steam. The real-number control parameters specify a total problem time of 20 days, purge-initiation hydrogen concentration of 3.5%, and an interval of 120 s after the end of blowdown for the release of the Zr-H₂O reaction hydrogen. The compartment has 2×10^6 ft³; is initially composed of air and steam at 14.7 psia, 120 °F, and a relative humidity of 0.5; has a purge capacity of 150 cfm; and will receive 100% of the (1) the H₂ due to sump-water radiolysis and (2) the O₂ and H₂ dissolved in the primary coolant, which depend on subsequent specifications. The reactor (which is always in compartment one) parameters are self explanatory. The corrosion parameters specify that the compartment has (1) an aluminum component with an area of 25 000 ft² and thickness of 0.2 in. and (2) a zinc component with an area of 75 000 ft² and a thickness of 0.003 in. The corrosion rates are specified to vary with time based on four time entries with aluminum rates that vary from 20 000 to 500 mil/yr and zinc corrosion rates from 300 to 10 mil/yr. Small time steps are specified as suggested in Appendix A. Note that after zero time, the compartment temperatures specified will be the steam-saturation temperatures.

The Sample Problem 1 calculated results show that (1) at time zero, the compartment has standard-air nitrogen and oxygen concentrations with the initial humidity, (2) the temperature and steam content increase sharply over

the first time step printed because of the specified steam-saturation temperature, (3) the hydrogen increases sharply over the first time step printed because of the Zr-H₂O reaction, (4) the hydrogen due to metal corrosion rates decrease with time, (5) the nitrogen and oxygen moles increase at 6 days because the hydrogen concentration reaches 3.5% causing the purge to be initiated, and (6) a maximum hydrogen concentration of ~3.8% is reached at ~12.5 days.

Sample Problem 2

The integer-control parameters specify that there will be a recombiner, no additional case, no plotting, two compartments, two recirculation connections, recombiner operation initiated when the compartment one hydrogen concentration exceeds a specified value (which has no significance for this problem because an initiation time is specified), and no steam. The real-number control parameters specify a total problem time of 20 days, recombiner initiation at 8 days, recirculation fan initiation at 0.75 days, and an interval of 120 s after the end of blowdown for the release of the Zr-H₂O reaction hydrogen. The compartment volumes are 0.3×10^6 and 1.2×10^6 ft³, initially composed of air only at 14.7 psia; the temperatures are 135 and 90 °F; and compartment 2 will receive 100% of (1) the H₂ due to sump-water radiolysis and (2) the O₂ and H₂ dissolved in the primary coolant, which depend on subsequent specifications. One recirculation fan will transfer 100 cfm from compartment one to compartment two and the second fan will transfer 100 cfm from compartment two to compartment one. The reactor (which is always in compartment one) parameters are self explanatory. The corrosion parameters specify that compartments one and two both have an aluminum and a zinc component. The corrosion rates are specified to vary with time based on 10 time entries with a complicated variation of corrosion rates. A recombiner to remove 100 cfm from compartment one and return the recombined flow to compartment two is specified.

For Sample Problem 2, (1) the compartment one and two concentrations start toward a common value after the recirculation starts at 0.75 days, which is about when the compartment one hydrogen concentration reaches its maximum of ~3.8% and (2) the number of hydrogen and oxygen moles begins to decrease after the recombiner is initiated at 8 days.

LISTING OF INPUT CARDS

COL-5	10	15	20	25	30	35	40	45	50	55	60	65	70	75	80
COGAP SAMPLE PROBLEM 1															
20.	2	1	0	1	0	1	1								
	2.E6	14.7	0.	3.5	120.		.5	120.	150.	100.	0.				
3651.		16000.	5000.		1.5			0.	0.						
.5		.5	10.		1.			50.	20.						
2															
1	1	25000.	.2												
1	2	75000.	.003												
4															
0.		20000.	300.		0.										
.02		1000.	100.		0.										
.05		1000.	50.		0.										
30.		500.	10.		0.										
4															
0.		.0002			500										
1.		.001			1000										
10.		.01			100										
30.		.01			50										
2															
0.		240.	40.		240.										
COGAP SAMPLE PROBLEM 2															
20.	3	0	0	2	2	1	0								
	.3E6	14.7	0.		.75			120.	0.	0.	0.	0.			
1	1.2E6	14.7	0.		90.			0.	0.	0.	100.	0.			
1	2	500.													
2	1	500.													
4000.		16000.	60000.		1.			0.	0.						
.5		.5	10.		1.			50.	20.						
4															
1	1	500.			.02										
1	2	50000.			.001										
2	1	100.			.02										
2	2	70000.			.001										
10															
0.		375.	2.8		0.										
.02083		1280.	13.5		0.										
.06944		2063.	23.1		0.										
.11574		2344.	27.5		0.										
.17361		2344.	27.5		0.										
.34722		1875.	19.4		0.										
.57870		1280.	14.4		0.										
1.1574		880.	8.8		0.										
2.3148		580.	4.9		0.										
30.		375.	2.8		0.										
4															
0.		.001			100			0							
1.		.01			100			0							
10.		.01			500			0							

LISTING OF INPUT CARDS

COL-5	10	15	20	25	30	35	40	45	50	55	60	65	70	75	80
		30.	.01		50		0								
2															
1	0.	240.			40.		240.								
1	2	100.													

Fig. B-1
Listing of input cards for Sample Problems 1 and 2.

---- INPUT DATA ----
(CASE 1)

CONTRDL PARAMETERS

ICON(1)	ICDN(2)	ICON(3)	ICON(4)	ICON(5)	ICON(6)	ICON(7)
2	1	0	1	0	1	1
CDN (1) DAYS	CON (2) DAYS	CON (3) PERCENT	CON (4) DAYS	CON (5) SEC		
20.00	0.00	3.50	0.00	120.00		

PARAMETERS FOR EACH VOLUME

VOLUME NO.	VOLUME CUFT	TOTAL PRES PSIA	P.N2 PRES PSIA	TEMPERATURE F	REL. HUM. =PSTM/PSAT	PUR. RATE CFM	FRC FRACTION	N2 AD. RATE CFM
1	2000000.00	14.700	0.0000	120.0	.50	150.00	100.00	0.00

R. COOLANT PARAMETERS

REACTOR POWER (MWT)	=	3651.00	REACTOR OPERATING TIME (HRS)	=	16000.00
ZIRCONIUM WEIGHT (LBS)	=	5000.00	ZIR-WATER REACTION, PER-CENT	=	1.50
O2 DISSOLVED IN PRI. COOL. (LB-MOLE)=		0.00	H2 DISSOLVED IN PRI. COOL. (LB-MOLE)=		0.00
G(H) IN CORE SOLUTION(MOLE/100 EV)=		.50	G(H) IN SUMP SOLUTION(MOLE/100 EV)=		.50
O/D NRG ABS. BY CORE WATER	=	10.00	O/O SOLID NRG ABS. BY SUMP WATER	=	1.00
O/O IOOINE NRG ABS. BY SUMP WATER	=	50.00	BLOWDOWN DURATION (SEC)	=	20.00

ALUMINUM ZINC AND COPPER CORROSION PARAMETERS
NO. OF ALU., ZINC AND COPPER COMPONENTS = 2

VOL. NO.	MATERIAL	SURF. AREA FT2	THICKNESS INCHES
1	1	2.5000E+04	2.0000E-01
1	2	7.5000E+04	3.0000E-03

CONT. MATERIAL CORROSION RATES AFTER LOCA
NO. OF PTS. IN TABLE = 4

TIME DAYS	AL COR RATE MIL/YR	Z. COR RATE MIL/YR	C. COR. RATE MIL/YR
0.00	20000.00	300.00	0.00
.02	1000.00	100.00	0.00
.05	1000.00	50.00	0.00
30.00	500.00	10.00	0.00

TIME STEP-SIZE TABLE
PTS. IN TABLE = 4

TIME DAYS	TIME INC. DAY	PRINT FREQ.	PLOT FREQ.
0.000	.00020	500	0
1.000	.00100	1000	0
10.000	.01000	100	0
30.000	.01000	50	0

CONTAINMENT TEMP. AFTER LOCA
TEMPS WILL BE SAT TEMP IF THERE IS STEAM
NO. OF PTS. IN TABLE = 2

TIME DAYS	TEMP. DEG-F
0.000	240.00
40.000	240.00

LEGEND FOR INPUT VARIABLES

- ICON(1) = 1 NO PURGE AND NO H2 RECOMBINER
- = 2 WITH PURGE
- = 3 WITH H2 RECOMBINER
- ICON(2) = 0 LAST CASE OR ONLY ONE CASE
- = 1 MULTIPLE CASE
- ***PLOTTING NOT AVAILABLE(9/80)***
- ICON(3) = 0 NO PLOT
- = 1 PLOTTING H2 GENERATION DUE TO RADIOLYSIS
- PLOTTING H2 GENERATION DUE TO METAL CORROSION
- PLOTTING H2 GENERATION DUE TO ZR-H2O REACTION
- PLOTTING TOTAL H2 GENERATION
- = 2 PLOTTING H2 CONCENTRATION IN EA. VOL.
- = 3 PLOTTING N2 CONCENTRATION IN EA. VOL.
- = 4 PLOTTING O2 CONCENTRATION IN EA. VOL.
- = 10 ALL THE ABOVE CASES WILL BE PLOTTED
- ***PLOTTING NOT AVAILABLE(9/80)***
- ICDN(4) = NUMBER OF VOLUMES
- ICON(5) = NUMBER OF JUNCTIONS
- ICON(6) = 0 THE AVERAGE VALUE OF ALL COMPARTMENT H2 CONCENTRATION WILL BE USED
- = X THE H2 CONC. IN X COMPT. WILL BE USED
- ICON(7) = 0 NO STEAM
- = 1 WITH STEAM BASED ON SATURATION TEMP
- CON(1) = PROBLEM END TIME, DAYS
- CON(2) = TIME AT WHICH PURGING OR H2 RECOMBINER STARTS, DAYS
- CON(3) = H2 CONCENTRATION AT WHICH PURGING OR H2 RECOMBINER STARTS
- CON(4) = TIME AT WHICH THE H2 RECIRCULATION FAN STARTS, DAYS
- CON(5) = DURATION FOR H2 RELEASED FROM ZR-H2O
- MAT(1) = H2 GENERATION MATERIALS
- = 1 ALUMINUM
- = 2 ZINC
- = 3 COPPER

NOTES - THIS LEGEND WILL BE PRINTED FOR THE FIRST CASE ONLY.
VOL. NO. 1 HOUSES REACTOR COOL. SYS.
INPUT 0.0 FOR PARTIAL N2 PRESSURE. UNLESS THE CONTAINMENT IS PRESSURIZED WITH N2 INITIALLY.

Fig. B-2
Description of input for Sample Problem 1.

---- OUTPUT DATA ----
(CASE 1)

VOL NO.	TIME DAYS	LB-MOLES					PER-CENT				PRES. PSIA	TEMP. F
		H2	N2	O2	STEAM	TOTAL	H2	N2	O2	STEAM		
1	0.000	0.00	3521.95	933.39	272.19	4727.53	0.00	74.50	19.74	5.78	14.70	120.0
1	.100	24.45	3521.95	936.75	6652.85	11135.99	.22	31.63	8.41	59.74	41.79	240.0
1	.200	34.34	3521.95	938.80	6652.85	11147.92	.31	31.59	8.42	59.88	41.84	240.0
1	.300	43.43	3521.95	940.45	6652.85	11158.66	.39	31.56	8.43	59.62	41.88	240.0
1	.400	52.04	3521.95	941.86	6652.85	11168.70	.47	31.53	8.43	59.57	41.91	240.0
1	.500	60.33	3521.95	943.12	6652.85	11178.25	.54	31.51	8.44	59.52	41.95	240.0
1	.600	68.38	3521.95	944.27	6652.85	11187.44	.61	31.48	8.44	59.47	41.98	240.0
1	.700	76.25	3521.95	945.32	6652.85	11196.36	.68	31.46	8.44	59.42	42.02	240.0
1	.800	83.97	3521.95	946.31	6652.85	11205.07	.75	31.43	8.45	59.37	42.05	240.0
1	.900	91.57	3521.95	947.25	6652.85	11213.61	.82	31.41	8.45	59.33	42.08	240.0
1	1.000	99.05	3521.95	948.14	6652.85	11221.98	.88	31.38	8.45	59.28	42.11	240.0
1	2.000	170.47	3521.95	955.53	6652.85	11300.79	1.51	31.17	8.46	58.87	42.41	240.0
1	3.000	237.73	3521.95	961.36	6652.85	11373.88	2.09	30.97	8.45	58.49	42.68	240.0
1	4.000	302.19	3521.95	966.30	6652.85	11443.29	2.64	30.78	8.44	58.14	42.94	240.0
1	5.000	364.47	3521.95	970.67	6652.85	11509.92	3.17	30.60	8.43	57.80	43.19	240.0
1	6.000	409.81	3542.59	978.62	6652.13	11583.15	3.54	30.58	8.45	57.43	43.47	240.0
1	7.000	423.59	3598.60	992.86	6652.13	11667.17	3.63	30.84	8.51	57.02	43.78	240.0
1	8.000	434.53	3648.88	1005.42	6652.13	11740.96	3.70	31.08	8.56	56.66	44.06	240.0
1	9.000	443.03	3694.01	1016.52	6652.13	11805.69	3.75	31.29	8.61	56.35	44.30	240.0
1	10.000	449.40	3734.51	1026.34	6652.13	11862.38	3.79	31.48	8.65	56.08	44.52	240.0
1	11.000	453.88	3770.89	1035.03	6645.67	11905.47	3.81	31.67	8.69	55.82	44.68	240.0
1	12.000	456.71	3803.54	1042.72	6645.67	11948.64	3.82	31.83	8.73	55.62	44.84	240.0
1	13.000	458.08	3832.85	1049.53	6645.67	11986.13	3.82	31.98	8.76	55.44	44.98	240.0
1	14.000	458.16	3859.16	1055.55	6645.67	12018.53	3.81	32.11	8.78	55.30	45.10	240.0
1	15.000	457.09	3882.77	1060.87	6645.67	12046.41	3.79	32.23	8.81	55.17	45.21	240.0
1	16.000	455.01	3903.96	1065.58	6645.67	12070.22	3.77	32.34	8.83	55.06	45.30	240.0
1	17.000	452.03	3922.98	1069.74	6645.67	12090.42	3.74	32.45	8.85	54.97	45.37	240.0
1	18.000	448.26	3940.06	1073.40	6645.67	12107.38	3.70	32.54	8.87	54.89	45.44	240.0
1	19.000	443.77	3955.38	1076.63	6645.67	12121.45	3.66	32.63	8.88	54.83	45.49	240.0
1	20.000	438.65	3969.14	1079.48	6645.67	12132.94	3.62	32.71	8.90	54.77	45.53	240.0
1	20.010	438.60	3969.27	1079.50	6645.67	12133.04	3.61	32.71	8.90	54.77	45.53	240.0

H2 GENERATION DUE TO DIFFERENT SOURCES (SCF)

VOLUME	TIME	ZIR-H2D	RAD.	METAL	TOTAL
1	0.000	0.00	0.00	0.00	0.00
1	.100	637.86	2596.74	6215.88	9450.48
1	.200	637.86	4176.53	8458.88	13273.27
1	.300	637.86	5452.02	10697.91	16787.79
1	.400	637.86	6547.75	12932.95	20118.56
1	.500	637.86	7521.00	15164.02	23322.88
1	.600	637.86	8405.52	17391.11	26434.49
1	.700	637.86	9223.06	19614.22	29475.14
1	.800	637.86	9988.27	21833.35	32459.48
1	.900	637.86	10711.37	24048.51	35397.73
1	1.000	637.86	11398.31	26255.27	38291.43
1	2.000	637.86	17112.68	48148.17	65898.71
1	3.000	637.86	21620.76	69643.27	91901.89
1	4.000	637.86	25443.40	90740.58	116821.83
1	5.000	637.86	28816.95	111440.08	140894.89
1	6.000	637.86	31876.25	131741.79	164255.90
1	7.000	637.86	34703.80	151645.70	186987.36
1	8.000	637.86	37352.45	171151.80	209142.11
1	9.000	637.86	39857.42	190260.11	230755.39
1	10.000	637.86	42243.08	208970.63	251851.56
1	11.000	637.86	44526.43	227281.55	272445.83
1	12.000	637.86	46720.81	245194.67	292553.34
1	13.000	637.86	48836.04	262709.99	312183.89
1	14.000	637.86	50879.79	279827.52	331345.16
1	15.000	637.86	52858.24	296547.25	350043.34
1	16.000	637.86	54776.50	312869.17	368283.53
1	17.000	637.86	56638.87	328793.30	386070.02
1	18.000	637.86	58449.06	344319.63	403406.54
1	19.000	637.86	60210.31	359448.16	420296.33
1	20.000	637.86	61925.51	374178.89	436742.26
1	20.010	637.86	61942.43	374324.19	436904.48

Fig. B-3
Calculated results for Sample Problem 1.

---- INPUT DATA ----
(CASE 2)

CONTROL PARAMETERS

ICON(1)	ICON(2)	ICON(3)	ICON(4)	ICON(5)	ICON(6)	ICON(7)
3	0	0	2	2	1	0
CDN (1) DAYS	CDN (2) DAYS	CDN (3) PERCENT	CDN (4) DAYS	CDN (5) SEC		
20.00	8.00	0.00	.75	120.00		

PARAMETERS FOR EACH VOLUME

VOLUME NO.	VOLUME CUFT	TOTAL PRES PSIA	P. N2 PRES PSIA	TEMPERATURE F	REL. HUM. =PSTM/PSAT	PUR. RATE CFM	FRC FRACTION	N2 AD. RATE CFM
1	300000.00	14.700	0.0000	135.0	0.00	0.00	0.00	0.00
2	1200000.00	14.700	0.0000	90.0	0.00	0.00	100.00	0.00

JUNCTION PARAMETERS

VOL(I)	VOL(J)	FLOW RATE
1	2	500.00
2	1	500.00

R. COOLANT PARAMETERS

REACTOR POWER (MWT)	•	4000.00	REACTOR OPERATING TIME (HRS)	=	16000.00
ZIRCONIUM WEIGHT (LBS)	•	60000.00	ZIR-WATER REACTION, PER-CENT	=	1.00
O2 DISSOLVED IN PRI. COOL. (LB-MOLE)	=	0.00	H2 DISSOLVED IN PRI COOL. (LB-MOLE)	=	0.00
G(H) IN CORE SOLUTION(MOLE/100 EV)	=	.50	G(H) IN SUMP SOLUTION(MOLE/100 EV)	=	.50
O/O NRG ABS. BY CORE WATER	=	10.00	O/O SOLID NRG ABS. BY SUMP WATER	=	1.00
O/O IOOINE NRG ABS. BY SUMP WATER	=	50.00	BLOWDOWN DURATION (SEC)	=	20.00

ALUMINUM, ZINC AND COPPER CORROSION PARAMETERS
NO. OF ALU., ZINC AND COPPER COMPONENTS = 4

VOL. NO.	MATERIAL	SURF. AREA FT2	THICKNESS INCHES
1	1	5.0000E+02	2.0000E-02
1	2	5.0000E+04	1.0000E-03
2	1	1.0000E+02	2.0000E-02
2	2	7.0000E+04	1.0000E-03

CONT. MATERIAL CORROSION RATES AFTER LOCA
NO. OF PTS. IN TABLE = 10

TIME DAYS	AL. COR RATE MIL/YR	Z. COR. RATE MIL/YR	C. COR. RATE MIL/YR
0.00	375.00	2.80	0.00
.02	1280.00	13.50	0.00
.07	2063.00	23.10	0.00
.12	2344.00	27.50	0.00
.17	2344.00	27.50	0.00
.35	1875.00	19.40	0.00
.58	1280.00	14.40	0.00
1.16	880.00	8.80	0.00
2.31	580.00	4.90	0.00
30.00	375.00	2.80	0.00

CONTAINMENT TEMP. AFTER LOCA
NOTE-THESE TEMPS WILL BE SAT TEMP IF THERE IS STEAM
NO. OF PTS. IN TABLE = 2

TIME DAYS	TEMP. DEG-F
0.000	240.00
40.000	240.00

TIME STEP-SIZE TABLE
PTS. IN TABLE = 4

TIME DAYS	TIME INC. DAY	PRINT FREQ.	PLOT FREQ.
0.000	.00100	100	0
1.000	.01000	100	0
10.000	.01000	50	0
30.000	.01000	50	0

JUNCTION PARAMETERS FOR H2 RECOMBINER
NO. OF JUNCTIONS FOR RECOM. = 1

VOL(I)	VOL(J)	FLOW RATE CFM
1	2	100.00

Fig. B-4
Description of input for Sample Problem 2.

APPENDIX C

DECAY ENERGY PRODUCTION FOR RADIOLYSIS

This appendix describes the decay energy production source equations that are the bases for the H_γ , $H_{\gamma+\beta}$, and H_I expressions in Eqs. (4) and (5) used for the determination of water radiolysis. The decay energy production source equations used are

1. the fission product decay energy production given by Eq. (2) of Ref. 5,
2. the heavy element decay energy production due to U^{239} given by Eq. (3) of Ref. 5,
3. the heavy element decay energy production due to Np^{239} given by Eq. (4) of Ref. 5, and
4. the decay energy production due to I^{131} through I^{135} , which provides the H_I expression.

First, the total decay energy production (H_{tot}) is calculated to be the sum of the first three items above. The sump water decay energy production term $H_{\gamma+\beta}$ then is determined by subtracting the energy production due to iodine (H_I) from the total. The core water decay energy production term H_γ is simply one-half of $H_{\gamma+\beta}$. The above operations can be expressed in equation form by

$$H_{\gamma+\beta} = H_{tot} - H_I$$

$$H_\gamma = 0.5 \times H_{\gamma+\beta} = 0.5 \times H_{tot} - 0.5 \times H_I .$$

The combined energy available (H_{avail}) for radiolytic hydrogen production is then

$$\begin{aligned} H_{avail} &= H_{\gamma+\beta} + H_\gamma + H_I \\ &= H_{tot} - H_I + 0.5 \times H_{tot} - 0.5 \times H_I + H_I \\ &= 1.5 \times H_{tot} - 0.5 \times H_I . \end{aligned}$$

This shows that the COGAP decay energy production available for radiolytic hydrogen generation is about 50% greater than the actual generation presented in Ref. 5 (the H_I is 1 to 10% of H_{tot}). However, the energy used for radiolysis is modified by the user supplied fractions that determine the energy absorbed, as shown in the input description in Appendix A.

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