A KINETIC MODEL OF SODIUM-WATER REACTION APPLIED TO DYNAMIC SIMULATION OF LEAK DETECTION IN THE CORE COMPONENTS TEST LOOP

by



pr 639

ANL-75-22

D. Saphier

BASE TECHNOLOGY





ARGONNE NATIONAL LABORATORY, ARGONNE, ILLINOIS Prepared for the U. S. ENERGY RESEARCH AND DEVELOPMENT ADMINISTRATION under Contract W-31-109-Eng-38

DISTRIBUTION OF THIS DOCUMENT IS UNUMEED

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency Thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

DISCLAIMER

Portions of this document may be illegible in electronic image products. Images are produced from the best available original document.

The facilities of Argonne National Laboratory are owned by the United States Government. Under the terms of a contract (W-31-109-Eng-38) between the U.S. Energy Research and Development Administration, Argonne Universities Association and The University of Chicago, the University employs the staff and operates the Laboratory in accordance with policies and programs formulated, approved and reviewed by the Association.

MEMBERS OF ARGONNE UNIVERSITIES ASSOCIATION

The University of Arizona Carnegie-Mellon University Case Western Reserve University The University of Chicago University of Cincinnati Illinois Institute of Technology University of Illinois Indiana University Iowa State University The University of Iowa Kansas State University The University of Kansas Loyola University Marquette University Michigan State University The University of Michigan University of Minnesota University of Missouri Northwestern University University of Notre Dame The Ohio State University Ohio University The Pennsylvania State University Purdue University Saint Louis University Southern Illinois University The University of Texas at Austin Washington University Wayne State University The University of Wisconsin

-NOTICE-

This report was prepared as an account of work sponsored by the United States Government. Neither the United States nor the United States Energy Research and Development Administration, nor any of their employees, nor any of their contractors, subcontractors, or their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness or usefulness of any information, apparatus, product or process disclosed, or represents that its use would not infringe privately-owned rights. Mention of commercial products, their manufacturers, or their suppliers in this publication does not imply or connote approval or disapproval of the product by Argonne National Laboratory or the U. S. Energy Research and Development Administration.

> Printed in the United States of America Available from National Technical Information Service U. S. Department of Commerce 5285 Port Royal Road Springfield, Virginia 22161 Price: Printed Copy \$5.00; Microfiche \$3.00

Distribution Category: LMFBR Sodium Technology (UC-79a)

ANL-75-22

ARGONNE NATIONAL LABORATORY 9700 South Cass Avenue Argonne, Illinois 60439

A KINETIC MODEL OF SODIUM-WATER REACTION APPLIED TO DYNAMIC SIMULATION OF LEAK DETECTION IN THE CORE COMPONENTS TEST LOOP

by

D. Saphier*

NOTICE This report was prepared as an account of work sponsored by the United States Government. Neither the United States nor the United States Energy Research and Development Administration, nor any of their employees, nor any of their contractors, subcontractors, or their employees, makes any hability or responsibility for the accuracy, completeness or usefulness of any information, apparatus, product or process disclosed, or represents that its use would not infringe privately owned rights.

July 1976



*On leave from the Israel Atomic Energy Commission Soreq Nuclear Research Centre

which and the provided with the second with

TABLE OF CONTENTS

.

	·	Page				
ABSI	TRACT	9				
I.	INTRODUCTION					
II.	THE CCTL LEAK-DETECTION EXPERIMENTAL SETUP	10				
III.	THE KINETICS OF SODIUM-WATER INTERACTIONS	12				
	A. The Sodium-Water Reactions	12				
	B. Hydrogen Equilibrium Concentration in Sodium	14				
	C. Decomposition Rate of Sodium Hydroxide	14				
	D. Dissociation Pressure of Sodium Hydride	15				
	E. Hydrogen Absorption by Sodium	15				
	F. Decomposition Rate of Sodium Hydride	16				
	G. Kinetic Equations	16				
IV.	DYNAMICS OF SODIUM-WATER REACTION-PRODUCT PROPAGATION	17				
	A. Sodium Flow and Concentration Changes	17				
	B. Hydrogen Partial Pressure in the Cover Gas	18				
	C. Hydrogen-gas Migration	19				
	D. Dynamics of a Pipe Segment	20				
V.	THE COLD TRAP	20				
	A. Cold-trap Efficiency	21				
	B. Cold-trap Dynamics	21				
	C. Solubility of Reaction Products	21				
VI.	DETECTORS	22				
VII.	A TYPICAL DATA SET TO BE USED WITH THE SIMULATION .	22				
VIII.	SUMMARY OF ASSUMPTIONS	27				

TABLE OF CONTENTS

			Page
IX.	SA	MPLE CALCULATIONS	29
	A.	Changes in Reaction-product Concentration as a Result of a Short, 0.075-1b Leak	29
	В.	Changes in Reaction-product Concentration as a Result of a 70-sec, 0.0001-lb/sec Leak	30
	C.	Effect of Changing Flow Rate	32
	D.	Simulation of a Tightly Coupled Loop	37
	E.	Effect of Cold-trap Operation	40
	F.	Effect of Different Reaction Rates	41
	G.	Effect of Leak Location	42
x.	ΕX	PERIMENTAL VERIFICATION	42
XI.	SU	MMARY AND CONCLUSIONS	44
API	PEN	DIXES	
	Α.	Mathematical Model Used in CCTL Dynamic Simulation Program (CCTL-DYSP)	47
		 An Ideal Mixing Plenum. Node with Cover Gas. Pipe Node and Generating Delay Functions Cold Trap. Detectors 	47 49 50 50 51
	в.	Description of CCTL-DYSP	53
	с.	Listing of CCTL-DYSP	55
	_		70

D,	\mathbf{Th}	e Input Data; How to Run CCTL-DYSP	78
	1.	Title	78
	2.	INLIST	78
	3.	PARM	79
	4.	DTCTR	80
	5.	Print-Plot Data	81
	6.	Sample Input Data Set	82
ACKNO	WL	EDGMENTS	84
REFER	EN	CES	85

LIST OF FIGURES

Title	е

No.

1.	Schematic Description of CCTL Loop	11
2.	CCTL Schematics for Simulation Program	11
3.	Transient Hydrogen Concentrations at Node 6, End of Pipe 49, in Detector 1, Resulting from a Steam Injection of 0.015 lb/sec for 5 sec from Injector I4 at Node 16	29
4.	Transient Hydrogen Concentrations at Nodes 16 and 23, End of Pipe 47, in Detector 3, Resulting from a Steam Injection of 0.015 lb/sec for 5 sec from Injector I4 at Node 16	30
5.	Transient Concentrations of Reaction Products Resulting from Steam Injection of 0.015 lb/sec for 5 sec from Injector I4 at Node 16	31
6.	Oxygen Concentration at Node 6 as Monitored by Oxygen Detector No. 2 Resulting from Steam Injection of 0.015 lb/sec for 5 sec at Injector I4	31
7.	Transient Hydrogen Concentrations at Nodes 16 and 23, End of Pipe 47, in Detector 3, Resulting from a Steam Injection of 0.001 lb/sec for 70 sec at Injector I4 and Node 16; Sodium Flow Rate of 800 gal/min at 940°F (504°C), without Cold Trapping	32
8.	Transient Concentrations of Reaction Products Resulting from a Steam Injection of 0.001 lb/sec for 70 sec at Injector I4; Sodium Flow Rate of 800 gal/min at 940°F (504°C), without Cold Trapping	33
9.	Response of Hydrogen Detectors to a Steam Injection of 0.001 lb/sec for 70 sec at Injector I4; Sodium Flow Rate of 800 gal/min at 940°F (504°C), without Cold Trapping	33
10.	Transient Hydrogen Concentrations at Nodes 1, 16, and 27 Resulting from a Steam Injection of 0.001 lb/sec for 70 sec at Injector I4; Sodium Flow Rate of 800 gal/min at 940°F (504°C), without Cold Trapping	34
11.	Response of Hydrogen Detector No. 1 at Different Sodium Flow Rates, to a Steam Injection of 0.001 lb/sec for 70 sec from Injector 14	34
12.	Response of Hydrogen Detector No. 3 to a Steam Injection of 0.001 lb/sec for 70 sec at Injector I4, during Sodium Flow at 300 anm	25
13.	Response of Hydrogen Detector No. 3 to a Steam Injection of 0.001 lb/sec for 70 sec at Injector I4, during Sodium Flow at	55
	465 gpm	35

LIST OF FIGURES

Title

<u>No</u> .	Title	Page
14.	Response of Hydrogen Detector No. 3 to a Steam Injection of 0.001 lb/sec for 70 sec at Injector I4, during Sodium Flow at 630 gpm	36
15.	Response of Hydrogen Detector No. 3 to a Steam Injection of 0.001 lb/sec for 70 sec at Injector I4, during Sodium Flow at 800 gpm	36
16.	Transient Hydrogen Concentration in a Tightly Coupled Loop at Pump Node 1 Resulting from a Steam Injection of 0.015 lb/sec for 5 sec into Sodium at 800 gpm and 940°F (504°C), at Injector 14	37
17.	Transient Hydrogen Concentrations in a Tightly Coupled Loop Resulting from a Steam Injection of 0.015 lb/sec for 5 sec at Injector I4, at 800 gpm and 940°F (504°C)	38
18.	Response of Hydrogen Detectors in a Tightly Coupled Loop Resulting from a Steam Injection of 0.015 lb/sec for 5 sec at Injector I4	38
19.	Transient Hydrogen Concentrations in a Tightly Coupled Loop Resulting from a Steam Injection of 0.015 lb/sec for 5 sec at Injector I4	39
20.	Transient Concentrations of Reaction Products in a Tightly Coupled Loop Resulting from a Steam Injection of 0.015 lb/sec for 5 sec at Injector I4	39
21.	Effect of Cold-trap Operation on Hydrogen Concentration in the Pump Segment	41
22.	Effect of Cold-trap Operation on Hydrogen Concentration in the CCTL Vessel	41
23.	Effect of Cold-trap Operation on Hydrogen Detector Monitoring the Steam-generator Outlet.	41
24.	Effect of Cold-trap Operation on Na ₂ O Concentration in the CCTL Vessel	41
25.	Change in Cover-gas Hydrogen Concentration When Hydrogen- disengagement Half-life is Reduced by a Factor of 1000	42
26.	Response of Hydrogen Detector No. 3 to a Steam Injection of 0.01 lb/sec for 5 sec from Two Different Injectors	43
27.	Transient Hydrogen Concentrations Resulting from Steam Injection of 0.01 lb/sec for 5 sec from Two Different Injectors	43

LIST OF FIGURES

<u>No</u> .	Title	Page
28.	Effect of Cold-trap Operation on Na ₂ O Concentration in CCTL Vessel	44
29.	Changes in Cover-gas Hydrogen Concentrations When Hydrogen- disengagement Half-life Is Reduced by a Factor of 1000	45
B.1.	Simplified Schematic Flowchart of CCTL-DYSP	53

LIST OF TABLES

No.	Title	Page
I.	Description of CCTL Experiment by Segments	23
II.	Initial Concentration of Reaction Products in Different Segments of CCTL	24
III.	Leak Distribution to Various Reactions and Reaction Products	25
IV.	Some Constant Parameters of the System	25
v.	Flow Distribution in CCTL	25
VI.	Water-leak Description for Experiment 1 Run 24	26
VII.	Description of Detector Connections for Experiment 1 Run 24	26

A KINETIC MODEL OF SODIUM-WATER REACTION APPLIED TO DYNAMIC SIMULATION OF LEAK DETECTION IN THE CORE COMPONENTS TEST LOOP

by

D. Saphier

ABSTRACT

A detailed model for the CCTL steam-generator leakdetection simulation was developed to predict the hydrogenand oxygen-detector response during a series of experiments to be performed at ANL. The detailed kinetic equations for the sodium-water interaction are given, as well as the assumptions made in assessing the various reactivity rates and hydrogengas migration in the sodium toward a free surface in contact with the cover gas. A dynamic model was developed describing concentration changes as a result of primary and secondary sodium reactions, sodium flow through the system piping, mixing processes in various plenum elements, cold-trap operation, cover-gas pressure changes, and water leaks. A computer program CCTL-DYSP has been written in which the dynamic model was simulated to obtain the concentration of the different reaction products as functions of time for any segment of the CCTL system. A generalized approach was used in the modeling and programming procedures, so that only the input data have to be changed in order to analyze different experiments and different system configurations. With minor changes, the computer program can be adapted to simulate leak detection in the CRBR. Some representative results are included in the report, and qualitatively they are in agreement with similar results published elsewhere. Some experimental results also became available recently, and they are in good agreement with the simulated concentrations.

I. INTRODUCTION

The hazard to LMFBR steam generators from small water leaks has long been recognized and has been the subject of several theoretical and experimental studies.¹⁻¹² Large water leaks in a superheater or evaporator will lead to a spontaneous violent reaction and to subsequent partial or complete destruction of the steam generator. Small leaks, if permitted to continue during a period sufficiently long, will produce corrosive agents that cause destructive wastage of the steam-generator tubing and finally result in "secondary" large leaks with extensive damage. It is, therefore, of utmost importance to detect the small leaks and their location so that the plant can be shut down before significant damage occurs.

Accordingly, an experimental leak-detection program¹ is underway in the Argonne Core Components Test Loop (CCTL) to evaluate methods for small-leak detection. The purpose of this experimental program is to evaluate the most efficient means for detecting water-to-sodium leaks in the range of 10^{-7} - 10^{-3} lb/sec and to gather enough experimental data on the leak-detection methods so that they can be applied to the Clinch River Breeder Reactor (CRBR). A series of experiments, as described in Ref. 1, to simulate water leaks in the CRBR heat exchangers will be performed. These experiments will be carried out under different flow rates, sodium temperatures, leak rates, and leak positions.

The purpose of the present study is to develop a mathematical model for the CCTL leak-detection experiment, and to set up a simulation program capable of solving the model equations in order that the leak-detector response can be predicted with reasonable accuracy. The modeling and the program are set up in a general way so that the CCTL experiment is a particular case. The computer program is modular and with minor changes can be applied to the simulation of other systems having water leaks into a sodium loop.

Several investigators^{1,6,8,10,12} have formulated general relationships between the size of the water leak and the quantity of hydrogen to be found in sodium after steady-state conditions are established. However, these relationships are usually system-dependent. In contrast, the mathematical model for the CCTL leak-detection experiment was developed from basic principles of conservation and the kinetic equations of the chemical reactions. Where certain basic parameters, such as reaction rates and hydrogen-gas disengagement rates, were not well known, reasonable assumptions were introduced. These assumptions can later be checked and improved by appropriate experiments. With this approach, the simulation program is rendered systemindependent and can easily be expanded to simulate leak detection in the CRBRP or other sodium systems.

II. THE CCTL LEAK-DETECTION EXPERIMENTAL SETUP

The Core Components Test Loop (CCTL) as well as the leak-detection experimental program are described in Ref. 1. Briefly, the CCTL is a large isothermal sodium loop, as is shown schematically in Fig. 1. The sodium is circulated through the main loop by a mechanical pump having a capacity of 800 gpm. The major component is a large sodium tank within which a simulated module of an CRBRP steam generator is placed. The water and steam pipes are simulated by solid stainless steel rods of the same diameter as the actual pipe. Water leaks are simulated by steam injections made directly into the module.



Fig. 1. Schematic Description of CCTL Loop

At several points in the system, sample lines direct a small fraction of the flow to various types of hydrogen and oxygen detectors. Among others,



Fig. 2. CCTL Schematics for Simulation Program

in-sodium hydrogen-diffusion, cover-gas hydrogen-diffusion, and electrochemicaloxygen meters are used. A bypass flow also passes to a purifying system, a cold trap, in which the impurities are removed from the sodium by precipitation. The bypass flows are governed by a series of valves and EM pumps, as shown in Fig. 1.

A schematic diagram of the CCTL leak-detection experiment, presenting features of importance to the mathematical modeling, is shown in Fig. 2. The CCTL system is divided into segments, each being considered as a lumped-parameter node. Two basic types of segments are used: (1) a mixing plenum, in which ideal mixing is assumed; and (2) pipes in which a pure delay and secondary reactions are assumed.

The steam-generator segments, nodes 6-22, are mixing-plenum segments

each having two baffle plates as a physical boundary. The flow between the segments is forced around the simulated tubes and the periphery of the baffle plate so that the total mixing is a good assumption for these segments. Steam injection points are designated as I1-I8.

Nodes 25-27 are the CCTL vessel segments and contain large volumes of sodium. Node 1 (the pump) and node 27 (the upper vessel section) are in contact with the cover gas, and hydrogen can leave sodium through these segments.

Node 42 is the cold trap where hydrogen and oxygen are removed from the system by cooling and precipitation.

In Fig. 2, detectors are connected to nodes 6, 23, and 25, and the covergas plenum; the other nodes depicted are pipe nodes.

The total flow through the system as it leaves the pump is designated as WS; constant flow is assumed. There is a small sodium bypass flow WEX from node 3 to node 22. Flow from node 7 to node 6 is equal to bypass flow WT1 to the detectors connected to pipe node 49. Other flows leaving the main flow are WT3 and WT4, detector flows, and WCT, the cold-trap flow. All bypass flows to the detectors return to the system through upper sodium node 27 in the CCTL vessel. In the version of the program given in Appendix C, up to 50 segments having sodium flow and sodium-water reactions can be simulated.

The <u>CCTL</u> <u>DY</u>namic <u>Simulation</u> <u>Program</u> (CCTL-DYSP) is based on the above schematic description of the system. The computer code is described in Appendix B. In the program, a mass and concentration balance for each segment shown in Fig. 2 is performed, using the kinetic and the dynamic equations developed in Secs. III and IV.

Simulation of slow transients must include the influence of cold trapping on the hydrogen and oxygen concentration in the system. Details on cold-trap dynamics appear in Sec. V.

Finally, the detector response is simulated by accounting for the hydrogen and oxygen diffusion through the detectors, and the appropriate time delays in the instrumentation piping.

III. THE KINETICS OF SODIUM-WATER INTERACTIONS

A. The Sodium-Water Reactions

When physical contact is made between sodium and water, with an excess of water, a spontaneous violent reaction occurs, producing sodium hydroxide and hydrogen:

$$Na + H_2O \rightarrow NaOH + \frac{1}{2}H_2(g). \tag{1}$$

However, under small-leak conditions prevailing in steam generators, the ratio of sodium to water is of the order of 10^6 and additional reactions take place:

$$2Na + H_2O \rightarrow NaOH + NaH; \tag{2}$$

$$4Na + H_2O \rightarrow 2NaH + Na_2O; \tag{3}$$

$$2Na + H_2O \rightarrow Na_2O + H_2. \tag{4}$$

The relative fraction of water participating in each of these reactions is dependent on the quantity of water introduced by the leak, the sodium temperature, and the sodium pressure. However, no numerical values were reported in the literature as to the quantity of water going into any of the four above reactions.

Therefore, in the present study, it was assumed that the above reactions are instantaneous and the fraction of water associated with each reaction is K1, K2, K3, and K4, respectively, and that

$$K_1 + K_2 + K_3 + K_4 = 1. (5)$$

Accordingly, when Q moles of water leak into sodium, four reaction products are generated with the following distribution:

$$Q(0.5 K_1 + K_4)$$
 moles of H_2 ; (6)

 $Q(K_1 + K_2)$ moles of NaOH; (7)

 $Q(K_1 + 2K_3)$ moles of NaH; (8)

$$Q(K_3 + K_4)$$
 moles of Na₂O. (9)

These products are predominantly dissolved and entrained by the rapid turbulent sodium flow. However, a fraction of the hydrogen is entrained as bubbles rather than dissolved in the liquid sodium. These bubbles will either diffuse and dissolve in the fluid, or escape into the cover gas.

Some of the products formed in the primary reactions are unstable at the temperatures prevailing in a steam generator or in the CCTL. The NaH and NaOH are dissociated according to the equations

$$Na + NaOH \rightarrow Na_2O + \frac{1}{2}H_2$$
(10)

and

$$NaH \neq Na + \frac{1}{2}H_2. \tag{11}$$

Thus, it is apparent that the ultimate products of the sodium-water reaction are predominantly hydrogen gas and sodium oxide, which can be detected by hydrogen and oxygen meters.

B. Hydrogen Equilibrium Concentration in Sodium

In systems under equilibrium conditions, some of the hydrogen dissolved in sodium escapes to the cover gas and is found to have a partial pressure P_H , independent of the cover gas pressure (usually argon). The equilibrium relation between the hydrogen in the cover gas and hydrogen in sodium (either as hydrogen or as NaH) is governed by the Sieverts' law:⁸

$$C_{\rm H} = K_{\rm S} P_{\rm H}^{1/2},$$
 (12)

where $C_{\rm H}$ is the hydrogen concentration in sodium (in mol/lb) and $K_{\rm S}$ is Sieverts' constant given by

$$K_{S} = 2.255 \times 10^{-6} \exp(1.9733 - 276.77/T_{K}),$$
 (13)

where K_S is in mol/lb-Torr^{1/2}, T_K is the temperature in degrees Kelvin, and P_H is the hydrogen partial pressure, in Torr (i.e., mm Hg).

C. Decomposition Rate of Sodium Hydroxide

In reactions 1 and 2, sodium hydroxide (NaOH) is formed. This product is unstable under normal reactor operating conditions and decomposes according to Eq. 10. In his experiments, which involved heating sodium with NaOD* at 500°C under vacuum, Fischer⁴ found that the reaction is of the first order according to

$$Rt = ln[C_0/(C_0 - C)]$$
(14)

where C_0 is the initial concentration, C is the concentration at time t, and R is the rate constant.

From the linear portion of the experimental curve, Fischer⁴ determined the rate constant to be

 $R = 0.0045 \text{ min}^{-1}$,

or in other terms, the half-life $\tau_{1/2}$ of NaOH is

^{*}D denotes deuterium.

 $\tau_{1/2} = 150$ min.

Therefore, $K_{NaOH} = 7.5 \times 10^{-5} \text{ sec}^{-1}$ was used in this study.

The hydroxide decomposition in sodium has also been treated by several authors,^{4,7,10} but none gave the temperature dependence of the reaction rate. In the present study, it was therefore assumed that the reaction rate is a constant.

D. Dissociation Pressure of Sodium Hydride

The partial pressure of hydrogen over NaH has been well established for a wide range of temperatures 1,4,9 and is given by

$$P_{dis} = \exp(26.71 - 14046/T_K), \tag{15}$$

where P_{dis} is the dissociation pressure, in mm Hg, and T_K is the temperature, in degrees Kelvin. Banus et al.¹¹ have shown that Eq. 15 is correct, even in dilute sodium solutions; therefore the equation was used in the present study.

E. Hydrogen Absorption by Sodium

Under vacuum, conditions at elevated temperatures, all the sodium hydride will be decomposed. However, hydrogen also will be absorbed by sodium if it is available in significant quantities in a cover-gas plenum over the sodium. Experiments by Longton³ reveal that if hydrogen is admitted over sodium at a pressure greater than the dissociation pressure, sodium hydride will form until the pressure decreases to a value equal to the dissociation pressure. The rate of absorption in terms of a pressure change ΔP_H is given by a simple parabolic law

$$\Delta \mathbf{P}_{\mathrm{H}} = \mathbf{K} (\mathbf{P}_{\mathrm{H}} - \mathbf{P}_{\mathrm{dis}})^{2}, \tag{16}$$

where P_H is the actual pressure in the cover gas, P_{dis} is the dissociation pressure, Δ indicates change in the variable, and K is the rate constant, which is temperature-dependent according to the Arrhenius equation

$$K = A \exp(-Q/RT).$$
(17)

From the semilogarithmic plots given by Longton,³ A and Q/R have been determined to be

$$A = 1.42 \times 10^9 \text{ sec}^{-1}$$
 and $Q/R = 11795^{\circ}K$.

Note, however, that at the temperatures of interest in the steam generator, the dissociation pressure of NaH is high [for 940° F (504° C), P_{dis} = 5670 mm-Hg]; hence, hydrogen from the cover-gas plenum is not expected to be absorbed in sodium.

F. Decomposition Rate of Sodium Hydride

Naud⁶ has reported some experiments to determine NaH dissociation rates. He reported large experimental errors. However, since these are the only rate constants available, they will be used in the present study. The values reported by Naud are

$$K(310^{\circ}C) = 0.05 \text{ min}^{-1}$$

and

$$K(280^{\circ}C) = 0.035 \text{ min}^{-1}.$$

On substituting these values into Eq. 17, we obtain the following expression for the rate of NaH dissociation:

$$R_2 = 0.597 \exp(-3883/T_K).$$
(18)

If, however, the partial pressure of hydrogen in the cover gas is equal to or greater than the NaH dissociation pressure, there will be no NaH dissociation. It is, therefore, assumed that both processes, i.e., NaH dissociation, and hydrogen absorption by the sodium and formation of sodium hydride, are governed by Eq. 16 and the combined rate constant is given by

$$K_{\text{NaH}} = R_{2} \left(\frac{P_{\text{dis}} - P_{\text{H}}}{P_{\text{dis}}} \right)^{2}.$$
(19)

G. Kinetic Equations

In Secs. A-F the various chemical reactions occurring when a small quantity of water is introduced into sodium were described. The dissociation equations of some of the products and their reaction rates were also given.

It is now possible to write the kinetic equations for a volume of sodium into which a leak of Q b/sec of water has been injected. These equations give the change in concentration of the reaction products as a function of time:

$$\dot{C}_{Nah} = \frac{d}{dt}C_{NaH} = (K_2 + 2K_3)\frac{Q}{M} - K_{NaH}C_{NaH},$$
 (20)

$$\dot{C}_{NaOH} = \frac{\dot{c}}{d^{\dagger}} (N_{aOH} = (K_1 + K_2) \frac{Q}{M} - K_{NaOH} C_{NaOH}, \qquad (21)$$

$$\dot{C}_{Na_2O} = \frac{d}{dt}C_{Na_2O} = (K_3 + K_4)\frac{Q}{M} + K_{NaOH}C_{NaOH},$$
 (22)

and

$$\dot{C}_{H_2} = \frac{d}{dt}C_{H_2} = (0.5K_1 + K_4)\frac{Q}{M} + 0.5(K_{NaH}C_{NaH} + K_{NaOH}C_{NaOH}),$$
 (23)

where C is the concentration (in mol/lb) of the different products, M is the sodium mass (in lb) in the calculated segment, K_{NaH} is given by Eq. 19, K_{NaOH} is a constant (in sec⁻¹), and Q is the leak rate (in mol/sec).

These equations are used in subsequent sections to develop the dynamic equations used in the simulation study.

IV. DYNAMICS OF SODIUM-WATER REACTION-PRODUCT PROPAGATION

The dynamic equations developed in this section are based mainly on mass balance applied to each segment and each product of the CCTL system. The equations are written in a general way so that the program can be adopted to other systems mainly by changing the input data. Some additional changes may be required due to differences in the physical-loop configurations.

A. Sodium Flow and Concentration Changes

The CCTL system is subdivided into several segment nodes as shown in Fig. 2. In a generalized node, the following processes occur:

- 1. Primary reactions resulting from water leak.
- 2. Secondary reactions.
- 3. Sodium flowing into and out of the segment.
- 4. Hydrogen gas entering or leaving the node.
- 5. Precipitation of reaction products.

The appropriate balance equations are

$$\frac{d}{dt}C_{1} = \frac{1}{M}\sum_{j} (W_{ij}C_{1ij} - W_{xj}C_{1}) + \dot{C}_{NaH}, \qquad (24)$$

$$\frac{d}{dt}C_{2} = \frac{1}{M}\sum_{j} (W_{ij}C_{2ij} - W_{xj}C_{2}) + \dot{C}_{NaOH},$$
(25)

$$\frac{d}{dt}C_{3} = \frac{1}{M}\sum_{j} (W_{ij}C_{3ij} - W_{xj}C_{3}) + \dot{C}_{Na_{2}O}, \qquad (26)$$

and

$$\frac{d}{dt}C_4 = \frac{1}{M}\sum_{j} (W_{ij}C_{4ij} - W_{xj}C_4) + \dot{C}_{H_2} - W_H/M, \qquad (27)$$

where

j = 1, ..., j for all inlet and outlet flows, i = inlet, x = exit, C_1 = concentration of NaH (in mol/lb) at any particular node, C_2 = concentration of NaOH (in mol/lb) at any particular node, C_3 = concentration of Na₂O (in mol/lb) at any particular node, C_4 = concentration of hydrogen (in mol/lb) at any particular node, W_{ij} = node inlet flow (in lb/sec) at the jth inlet, W_{xj} = node exit flow (in lb/sec) at the jth outlet, M = total mass of sodium (in pounds) in the node, W_H = net hydrogen gas (in mol/sec) leaving (or entering) the node,

and

 $\dot{C}_{NaH},\,\dot{C}_{NaOH},\,\dot{C}_{Na_2O}$, and \dot{C}_{H_2} are time derivatives given by Eqs. 20, 21, 22, and 23, respectively.

B. Hydrogen Partial Pressure in the Cover Gas

In the sodium loop of an LMFBR steam generator, as well as in the CCTL leak-detection experiment, the sodium may have a free surface with an inert cover gas in several places. Under leak conditions, hydrogen generated in the sodium will escape into the cover gas. If, for some reason, a high concentration of hydrogen or steam exists in the cover gas, it will be partially absorbed in the sodium flow.

In the CCTL experiment, the coolant contacts the cover gas in two places: the pump and the CCTL vessel. The amount of gas (in mol/sec) that can leave these nodes is $W_{\rm HP}$ and $W_{\rm HC}$ for the pump and the CCTL vessel, respectively. All cover-gas plena are connected through the expansion tank, and equal pressure is assumed to exist in each plenum.

The hydrogen partial gas pressure P_H is calculated from the ideal gas law PV = nRT:

$$W_{H} = W_{HP} + W_{HC}; \qquad (28)$$

$$\frac{\mathrm{dP}_{\mathrm{H}}}{\mathrm{dt}} = 554.4 W_{\mathrm{H}} T_{\mathrm{p}\ell} / V_{\mathrm{p}\ell}, \qquad (29)$$

where P_H is in mm Hg, W_H is in mol/sec; $T_{p\ell}$ is the temperature (in degrees Rankine), and $V_{p\ell}$ is the total plenum volume (in cubic feet).

C. Hydrogen-gas Migration

The quantity of hydrogen gas produced at the leak site is given by Eq. 6. This hydrogen can be in two forms; it can be either dissolved in the sodium or in the form of tiny bubbles. No information was found in the literature on whether any hydrogen bubbles are formed and what the fraction or sizes of these bubbles are. From the experiments performed so far there is, however, a strong indication that no bubbles are formed at the high temperatures prevailing in the heat exchanger, but some of the hydrogen might be produced in bubbles under low-temperature condition.

The conditions under which hydrogen bubbles are formed and their subsequent behavior in the system are the subject of ongoing theoretical and experimental investigations. In this study, it is assumed that if free hydrogen is formed during reactions at the leak site, it will be completely dissolved in the sodium. This assumption is well justified above 600° F (316°C) and will probably be increasingly erroneous as the temperature of the sodium in the CCTL experiment is lowered.

A model for the possible migration or diffusion of the dissolved hydrogen and its subsequent escape into the cover gas has been developed based on the following assumptions:

1. Dissolved hydrogen will diffuse from the sodium into the cover gas only when the partial pressure in the cover gas is less than the value governed by Sieverts' law (Eq. 12).

2. Hydrogen from the cover gas will enter the sodium only if the partial pressure of the cover gas is higher than the NaH dissociation pressure.

3. Independent hydrogen-gas migration occur only in parts of the system where very slow flow exists; otherwise the gas will be entrained in the sodium flow.

4. The gas will migrate only in the upward direction.

5. The rate at which the hydrogen migrates to the cover gas is determined by the difference between hydrogen concentration and the equilibrium value according to Seiverts' law:

$$W_{\rm H} = R_1 (C_{\rm H} - C_{\rm HS}) M \text{ for } C_{\rm H} > C_{\rm HS}.$$
 (30)

6. The rate constant R_1 , which governs the hydrogen disengagement rate, is assumed to be such that, if zero partial pressure of hydrogen exists in the cover gas, it will take $\tau_{1/2}$ for half the hydrogen necessary to establish equilibrium to leave the sodium node:

$$R_1 = (\ell_n 2) / \tau_{1/2} = 0.693 / \tau_{1/2}.$$
(31)

D. Dynamics of a Pipe Segment

Dynamic equations for a pipe containing M pounds of sodium flowing at W lb/sec are determined by the transit time τ , which is given by

$$\tau = M/W. \tag{32}$$

The concentration of any of the reaction products at time $t - \tau$ is given by

$$C' = C(t - \tau). \tag{33}$$

Hence, C' is the concentration of a reaction product τ seconds before it reaches the pipe exit.

There are no leaks in these pipe segments; therefore, only secondary reactions take place. The change in C', which was confined to the pipe segment during time τ , is obtained by the following single-step integration process:

$$\Delta C_1 = -K_{NaH} C_1' \tau , \qquad (34)$$

$$\Delta C_2 = -K_{\text{NaOH}} C_2^{\dagger} \tau, \qquad (35)$$

$$\Delta C_3 = K_{\text{NaOH}} C_2^{\dagger} \tau, \qquad (36)$$

and

$$\Delta C_4 = 0.5 (K_{NaH}C_1' + K_{NaOH}C_2')_{\tau}.$$
(37)

This is a coarse integration process and can be justified only because the secondary reaction-rate constants are very small.

The concentration of any of the reaction products at the exit of the pipe at time t is given by

$$C(t) = C' + \Delta C. \tag{38}$$

V. THE COLD TRAP

Impurities are removed from the sodium by cooling it to temperatures at which the solubility of some of the reaction products is reduced considerably. A small stream of the sodium is bypassed through a special heat exchanger called a cold trap. If the concentration of the impurities exceeds the amount that can be dissolved in sodium at the cold-trap temperature, the excess will precipitate.

A. Cold-trap Efficiency

Theoretically, the impurity concentration in sodium at the cold-trap outlet should be equal to its solubility at the cold-trap temperature. However, the operating characteristics of the cold trap change with time and flow rate, with consequent changes in its static efficiency, which is given by¹²

$$\beta = \frac{C_i - C_x}{C_i - C_{sat}},$$
(39)

where C_i and C_x are the impurity concentrations at the inlet and outlet, and C_{sat} is the saturation concentration for the cold-trap temperature.

B. Cold-trap Dynamics

In a dynamic system, the widely accepted concept of the static efficiency β cannot be used. Instead, a dynamic efficiency is defined by

$$M\frac{dC}{dt} = W_{ct}(C_{in} - C) - \beta_d(C_{in} - C_{sat}), \qquad (40)$$

where C is the average outlet concentration (in mol/lb), and $\beta_{\rm d}$ is the dynamic efficiency, given by

$$\beta_{d} = f(W_{ct}, T_{ct}), \qquad (41)$$

where W_{ct} is flow rate through the cold trap (in lb/sec), and M is the sodium content in the cold trap (in pounds). The exact dependence of β_d on the flow rate and other factors is presently unknown.

C. Solubility of Reaction Products

Available data on the solubility of hydrogen and oxygen in sodium have been summarized by Rodgers and Dutina.⁵ Their recommended values as function of temperature were used in this study.

For NaH,
$$C_{1sat} = \exp(13.97 - 6631.4/T_K)$$
. (42)

For Na₂O, C_{3sat} =
$$\exp(16.131 - 6493.3/T_K)$$
. (43)

The concentrations are given in ppm, and $\mathbf{T}_{\mathbf{K}}$ is the cold-trap temperature in degrees Kelvin.

VI. DETECTORS

The results of the CCTL leak-detection experiments will be available through reading and interpreting outputs from the hydrogen and oxygen detectors. Outputs from the hydrogen detectors will be proportional to the NaH and hydrogen concentrations, and outputs from the oxygen detectors will be proportional to the Na₂O concentration.

To predict the detector outputs, the simulation employs three parameters that characterize the detectors: (1) the time lag τ , which is the time for the tiny stream of sodium to reach the detecting apparatus; (2) the diffusion time constant θ of the detector, i.e., the time for hydrogen or oxygen to diffuse through the membrane until equilibrium is achieved between the measured sample stream and the detector interior; and (3) the proportionality or calibration constant of the detector.

The detector transfer function is given by

$$\frac{A}{C} = \frac{K_{d}e^{-S\tau}}{1+S\theta},$$
(44)

where A is the detector reading, C is the actual concentration, S is the Laplace-transform operator, and K_d is the proportionality constant.

VII. A TYPICAL DATA SET TO BE USED WITH THE SIMULATION

A data set that describes the CCTL system, the conditions at which the particular experiment is performed, and some initial conditions is given in Tables I-VII. Except for the explanatory titles, the tables are reproductions of CCTL-DYSP printouts of initial data used in a CCTL leak-detectionexperiment simulation.

Table I presents data describing the system segments, length, cross section, area, the total mass of sodium in each segment, and the flow through each segment. Table II shows the initial conditions in each segment. Table III gives some reaction parameters and how much of each reaction product is generated per mole of water leak. Table IV gives some system constants, and Table V gives the input flow values through various passages. Table VI shows the leak experiment for a particular run, and Table VII describes the detectors.

TABLE I Description of CCTL Experiment by Segments TYPE 0, not simulated, TYPE 1, mixing plenum,TYPE 2, a pipe segment, TYPE 3, plenum with cover gas; TYPE 4, segment with multiple entry, TYPE 5, segment with cover gas and multiple entry

***	****	*****	KUN # 24:	CCTLP LEAK	DETECTION
SE	EGM	TYPE SE	GMENT PARAM	ETERS	
		LENGTH	CROSS-AREA	MASS	FLOW
		<u>(ft)</u>	<u>(ft²)</u>	(16)	(Ib/sec)
1 7	* 3	1.000E 00	1.069E 00	5.583E 01	9.309E U1
5.	* 2	4.090E 01	9.893E-02	2.115E 02	9.309E 01
3 7	* 1	1.000E 00	3.395t-01	1./75E 01	9.309E 01
4 1	* 2	1.000E 01	9.8936-02	5.166E 01	9.297E 01
י כ	* 1	1.000E 00	2.12/E-01	1.1111 01	9.297E 01
6 7	*]	1.000E 00	1.490E 00	/ ./81E 01	5.018E=V1
/ '	* <u> </u> + 1		3.2400-01	4.6950 00	9.297E UJ
0,	* 1	4.1710-01	5.2406-01	6 804F 00	4 2 4 9 F 0 1
10 7	~ 1 + 1	4 588F=01	5 2406-01	7 7638 00	9.239E 01
11 5	* 1	7.788F=01	3-2401-01	1.515E 01	9-239E 01
12	* 1	8-546E=01	3.240E-01	1.446F 01	9.239E 01
13	* 1	7.7885-01	3.2401-01	1.518F 01	4.239F 01
14	* 1	7.221E-01	3.240E-01	1.2222 01	9.2548 01
15	* 1	7.221E-01	3.240E-01	1.2228 01	9.239E 01
16	* 1	7.788E-01	5.240E-01	1.318t 01	9.239E 01
17	* 1	8.546E-01	3.240E-01	1.446E 01	9.234E U1
18	* 1	7.768E-01	3.2406-01	1.518E 01	9.239E 01
19	* 1	4.588E-01	3.240E-01	7.7631 00	9.234E 01
20	* 1	4.021E-01	5.240E-01	0.805E 00	9.234E 01
21	* 1	4.171E-01	3.240E-01	1.057E 00	9.239E 01
22	* 4	3.889E-01	3.240E-01	6.580E 00	°.251E 01
23	* 1	1.000E 00	2.127E-01	1.111E 01	9.251E 01
24	* ?	2.890E 00	9.893E-02	1.493E 01	9.192E 01
25	* 1	1.000E 00	4.030E 00	2.1054 02	9.192E 01
26	* 1	2.083E 00	6.335E 00	0.891E 02	9.140E UI
21	ר * - ר	1.000E 00	1 5 3 5 - 01	2.3246 93	9.202E VI
20	* ~	1.900E 01 9.000E-01	1.5256=01	1. JI4C UC	9.202E 91
30	* 7	3 100E 01	1.5255-01	2 3708 02	9.309E 01
31 3	* 0	1.000E 00		0.0	0.0
32	* 0	1.000E 00	0.0	0.0	0.0
33 :	* 0	1.000E 00	0.0	0.0	J.U
34	* 0	1.000E 00	0.0	0.0	J.O
35	* U	1.000£ 00	0.0	0.0	J.O
36	* 0	1.000E 00	0.0	0.0	0.0
37 :	* 0	1.000E 30	0.0	0.0	J.J
38 :	* 0	1.000E 00	U.J	0.0	7.0
39 :	* 0	1.000E 00	0.0	0.0	0.0
40	* 0	1.000E 00	0.0	U.U	0.0
41	* 5	2.800E 01	2.4805-05	3.626F 00	4.0546-01
42	* 1	1.000E 00	3.2/6E 00	1./11E 02	4.0545-01
43	* 2 • •	1.600E 01	2.4805-05	2.0/2E 00	4.0545-01
44 :	* () + ^	1.600E 01	1.796E=U1	1.5010 02	0.0
45	× 0	0.0	0.0	J.V	0.0
40 // 7	∧ U + ⊃	U.U. 1 MEGE A1		2 4675 66	0.0 5.818F=01
4/	~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~	1.000C U1 7.687- 01	2 4805-03	7 1826 00	5.8185=01
40	- 2 + 2	1 267E 01		526F 00	5-818+=01
50	* 2	4.2266 01	2-4806-03	1.100F 01	5.818F=01
-0	·· 6.	HALEVE VI	C	TETOLE AT	

				CONCENTRAT	ION. MOL/LB	
SEGM	1	TYPE	C1-NAH	C2-NAOH	C3-NA20	C4-H2
1	*	3	1.418E-06	1.134E-08	2.561E-04	2.249E-06
5	*	2	1.418E-06	1.134E=08	2.561E-04	2.2491-06
3	*	1	1.418E-06	1.134E-08	2.561E-04	2.249E-06
4	*	5	1.418E-06	1.134E-08	2.561E=04	2.249E-06
5	*	1	1.418E-06	1.134E-08	2.561E=04	2.2498-06
6	*	1	1.418E-06	1.134E-08	2,561E-04	2.249E-06
7	*	1	1.418E-06	1.134E-08	2.561E-04	2.249E-06
8	*	1	1.418E-06	1.134E-08	2.561E-04	2.249E-06
9	*	1	1.418E-06	1.134E-08	2.561E-04	2.249E-06
10	*	1	1.418E=06	1.134E-08	2.561E=04	2.249E-06
11	*	1	1.418E-06	1.134E-08	2.501L-04	2.249E-06
12	*	1	1.418E-06	1.134E-08	2.561E-04	2.249E-06
13	*	1	1.418E-06	1.134E-08	2.561E=04	2.249E-06
14	*	1	1,418E-06	1.134E-08	2.561E-04	2.249E=06
15	*	1	1.418E-06	1.134E-08	2.561E = 04	2,249E-06
16	*	1	1,418E-06	1.134E-08	2.561E = 04	2.249E-06
17	*	1	1.418E-06	1.134E-08	2.561E-04	2.249E-06
18	*	1	1.418E-06	1.134E-08	2.561E - 04	2.249E-06
19	*	1	1.418E-06	1.134E-08	2.561E - 04	2.249E-06
20	*	1	1.418E-06	1.134E = 08	2.561E = 04	2.249E-06
21	*	1	1.418E=06	1.134E = 08	2.561E-04	2.249E-06
55	*	4	1,418E-06	1.134E = 08	2.561E - 04	2.249E-06
53	*	1	1.418E-06	1.134E-08	2.561E-04	2.249E-06
24	*	5	1.418E = 06	1.134E = 08	2.561E-04	2.249E=06
25	*	1	1.418E=06	1.134E = 08	2.561E-04	2.249E=06
56	*	1	1.418E=06	1.134E-08	2.561E=04	2.249E-06
27	*	5	1.418E-06	1.134E=08	2.561E-04	2.249E-06
28	*	2	1.418E-06	1.1348-08	2.561E=04	2.2491-06
29	*	4	1.418E-06	1.134E-08	2.561E=04	2.249E=06
50	*	2	1.418E=06	1.134E = 08	2.561E-04	2,2496-06
21	*	0	0.0	0.0	0.0	0.0
36	×	0	0.0	0.0	0.0	0.0
22	×.	0	0.0	0.0	0.0	0.0
26	×	0	0.0	0.0	0.0	0.0
30	2	0	0.0	0.0	0.0	0.0
27	Ŷ	0	0.0			0.0
J/ 10	Ŷ	0	0.0	0.0	0.0	0.0
10	÷	Ň	0.0	0.0	0.0	0.0
40	÷	0	0.0	0.0	0.0	0.0
41	÷	2	1 //18E_06	1 13/15-08	2 5615-04	2 2/195-06
<u>д</u> р	*	1	1 4186-06	1 1346-08	2 561E-04	2 2/195-06
42	*	2	1.4181-04	1.1441-08	2.5611-04	2.2495-06
44	*	0	0.0		0.0	
Δ5	*	ñ	0 0	0.0	0.0	0.0
46	*	õ	0.0	0_0	0.0	0.0
47	*	Ž	1.418F=06	1.134F=08	2.561E=04	2.249F=06
48	*	2	1.4186-06	1.154F=08	2.5616-04	2.2491-06
49	*	Ž	1.418F-06	1.134F=08	2.561F=04	2.249F=06
50	*	. 2	1.418E-06	1.134E+08	2.561E-04	2.249E-06
-		-				

TABLE II. Initial Concentration of Reaction Productsin Different Segments of CCTL

TABLE III. Leak Distribution to Various Reactions and Reaction Products

0.45	OF TH	LEAK	GUES	τu	NA+H20=NA	0 11	F1/2H2(G)
0.20	OF THE	E LEAK	GDES	TO	2NA+H2U=NA	OH	FNAH
0.25	UF TH	LEAK	GUES	τu	4NA+H20=2N	IAH-	ISAN4
0.10	OF TH	LEAK	GOES	TU	2NA+H20=NA	201	FH5
0.70	MOL O	THE	LEAK I	S TR	ANSFORMED	τu	NAH
0.65	MOL OF	THE	LEAK I	S TR	ANSFORMED	ΤU	NAUH
0.35	MOL U	THE	LEAK I	S TR	ANSFORMED	τũ	NA20
0.32	MOL OF	THE	LEAK I	S TR	ANSFORMED	ΤU	H2(G)

TABLE IV. Some Constant Parameters of the System

THE NAH DISSOCIATION PRESSURE IN MM-HG IS	3332.611
SODIUM TEMPERATURE IN (DEG=K) IS	755.22
SODIUM DENSITY IN (LBS/CUF) IS TOTAL WEIGHT OF SODIUM IN THE SYSTEM (LB)	52.22 4785.61
COVER GAS PLENUM VOLUME (LUF) COLD TRAP DYNAMIC EFFICIENCY (1/SEC) IS	40.00 0.2449E-02
NAH SATURATION CONC. AT CULD TRAF(MUL/LB) NAZO SATURATION CNC. AT CULD TRAF(MUL/LB)	0.8542E-06
TOTAL TRANSIT TIME IN CCTL (SEC) IS	46.87
SIEVERTS CÜNSTANT IN (MUL/(L&*TuRR**-2)) PARTIAL HYDROGEN PRESSURE IN COVER GAS (MM-HG)	0.1125E-02
PARTIAL ARGON PRESSURE IN COVER GAS (MM-HG)	800

TABLE V. Flow Distribution in CCTL (see Fig. 2 for explanation)

TOTAL	SODIUM	FLOw	IN	(LBS/SEC) 15	93.0872
				WCT	0.4654
				W] 1	0.5818
				WT2	0.0
				WT3	0.5818
				WT4	0.0
				WEX	0.1164
				W A	92.9709
				WX	92.3891
				WB	92.5054
				wC	91.9236
				WD	91.4582
				wE	92.6217
.				w R	93.0872

**************************************	TI LEAK DETEN	TION SIMULA	TIÚN. (.001 L	B/SEC AT INJ#4	DUR=70SEC	****
					• • • • • • • • • • • • • • • • • • • •	
LEAKAGE DATA FUR THIS CASE	ARE:					
FOR NUDE SEGMENT #	22	19	17	16	15	12
THE LEAKAGE IN MUL/SEC IS	0.0	0.0	0.Ù	0.3776E 00 (1.0	0.0
THE LEAK STARTS AT TIME -	10.00	10.00	10.00	10.00	10.00	10.00
THE LEAK IS TERMINATED AT	80.00	80.00	80.00	15.00	80.00	80.00

TABLE VI. Water-leak Description for Experiment 1 Run 24

TABLE VII. Description of Detector Connections for Experiment 1 Run 24

DETECTOR	NO	1	ÛF	TYPE	1	15	CUNECTED	TU	NUDE	49	HAS	۵	LAG	UF	10.00SEC	AND	A	DELAY	UF14.00SEC
DETECTOR	NO	2	ÛF	TYPE	2	IS	CUNECTED	ŢŨ	NÜDE	49	HAS	4	LAG	UF	12.00SEC	AND	A	DELAY	UF15.00SEC
DETECTUR	NŰ	3	υF	TYPÉ	1	15	CUNECTED	τu	NÜDE	47	HAS	A	LAG	ΰF	10.00SEC	AND	A	DELAY	OF14.00SEC
DETECTUR	NŬ	4	OF	TYPE	3	15	CUNECTED	τo	NUDE	27	HAS	۵	LAG	UF	1.00SEC	AND	A	DELAY	DF10.00SEC

Type I = Hydrogen Detector

Type 2 = Oxygen Detector

Type 3 = Hydrogen Detector in the Cover Gas

- 1. Reactions 1-4 are the only sodium-water reactions expected at the leak site.
- 2. As a result of a leak of 1 mol of water, the following reaction products will be generated instantaneously:

0.7 mol of NaH
0.65 mol of NaOH
0.35 mol of Na₂O
0.37 mol of H₂

- 3. The only secondary reactions taking place in the system are NaOH and NaH dissociation, as given by Eqs. 10 and 11.
- 4. The half-life of NaOH is 150 min.
- 5. The NaH dissociation pressure is given by Eq. 15:

 $P_{dis} = \exp(26.71 - 14046/T_K).$

- 6. If the system is at steady state for a long time, the hydrogen pressure in the cover gas will be in equilibrium with the hydrogen concentration in the sodium according to Sieverts' law.
- 7. Changes in the cover-gas hydrogen partial pressure are the result of hydrogen leaving the sodium according to the Sieverts' law and because of bubble transport from the leak site. Bubble transport occurs only at low temperatures and is assumed to be zero at the temperatures considered in this study.
- 8. The NaH dissociation rate is given by

$$K_2 = 0.597 \exp(-3883/T_K) \left(\frac{P_{dis} - P_H}{P_{dis}}\right)^2$$
.

- 9. Ideal mixing is assumed in all plenum segments.
- 10. Hydrogen diffusion through the system walls is neglected.
- 11. The hydrogen and oxygen detectors are of the diffusion type and can be characterized by the transfer function given in Eq. 44:

$$\frac{A}{C} = \frac{K_d e^{-S\tau}}{1 + S\theta}$$

12. Solubility of NaH in sodium is given by Eq. 42,

 $C_{NaH} = exp(13.97 - 6631.4/T_K).$

13. Solubility of Na₂O in sodium is given by Eq. 43,

$$C_{Na_2O} = \exp(16.131 - 6493.3/T_K).$$

- 14. Steady-state flow conditions prevail throughout the system; therefore, there is a constant sodium level in CCTL vessel and zero flow to the expansion tank.
- 15. The system temperature is constant; no heat transfer is accounted for.
- 16. Pressure gradients throughout the flow path and their possible effects on reaction rates are neglected.

IX. SAMPLE CALCULATIONS

The following sample calculations are intended to demonstrate various output features of the program rather than to predict the results of a particular CCTL experiment.

A. <u>Changes in Reaction-product Concentration as a Result of a Short</u>, 0.075-lb Leak

A short leak of 0.015 lb/sec, starting at 10 sec after simulation startup and terminating at 15 sec, was generated to initiate a transient in the CCTL system. The injection point was I4 (in the middle of the steam-generator module). The conditions are basically similar to those given in Tables I-VII, except for the leak size. The simulation was run for 100 sec, a sufficient time for the major transients to be terminated.

Figure 3 shows the hydrogen concentration in sodium as a function of time (1) at the leak-injection site (node 16); (2) at the stagnant part of the steam generator (node 6) through which there is a small (5-gal/min) samplingline flow; (3) at the end of the pipe leading to hydrogen detector No. 1; and (4) as given by the response of detector No. 1. The delays among the various nodes are clearly visible. The effect of mixing increases with distance from the injection node; therefore, the peaks observed during the transients are lower at the distant nodes.



Fig. 3. Transient Hydrogen Concentrations at Node 6, End of Pipe 49, in Detector 1, Resulting from a Steam Injection of 0.015 lb/ sec for 5 sec from Injector I4 at Node 16 (See Fig. 2)

Figure 4 shows the hydrogen concentration (1) at the steam-generator outlet plenum (node 23); (2) at the end of sampling line 47 leading from node 23 to the hydrogen detector No. 3; and (3) as given by the response of detector No. 3. For comparitive purposes, the hydrogen concentration at the injection node is also shown.



Fig. 4. Transient Hydrogen Concentrations at Nodes 16 and 23, End of Pipe 47, in Detector 3, Resulting from a Steam Injection of 0.015 lb/sec for 5 sec from Injector I4 at Node 16 (See Fig. 2)

Figure 5 shows the concentration of the four reaction products at node 27, which is in contact with the cover gas. Apart from differences in concentrations, which are the results of the assumption on how the sodiumwater reaction products split, the transient forms of the four curves are identical.

Figure 6 shows the oxygen concentration at node 6, as monitored by oxygen detector No. 2.

B. Changes in Reaction-product Concentration as a Result of a 70-sec, 0.0001-lb/sec Leak

This run simulated a proposed CCTL leak-detection experiment with a sodium flow rate of 800 gal/min at 940°F (504°C). Steam at 0.001 lb/sec was introduced at Injector I4 (see Fig. 2) 10 sec after simulation startup. The leak was terminated at 80 sec, and simulation was continued up to 600 sec. The cold trap was not in operation in this experiment.



Fig. 5 Transient Concentrations of Reaction Products Resulting from Steam Injection of 0.015 lb/sec for 5 sec from Injector I4 at Node 16 (See Fig. 2)



Fig. 6. Oxygen Concentration at Node 6 as Monitored by Oxygen Detector No. 2 Resulting from Steam Injection of 0.015 lb/ sec for 5 sec at Injector I4 (See Fig. 2)

Figure 7 shows the hydrogen concentration at the injection point (node 16), at node 23, at the end of pipe section 47, and at hydrogen detector No. 3. The delays in concentration changes among the various nodes are clearly seen.



Fig. 7. Transient Hydrogen Concentrations at Nodes 16 and 23, End of Pipe 47, in Detector 3, Resulting from a Steam Injection of 0.001 lb/sec for 70 sec at Injector I4 and Node 16 (See Fig. 2), Sodium Flow Rate of 800 gal/min at 940°F (504°C), without Cold Trapping

Figure 8 shows the concentrations of the four reaction products at node 27. A relatively fast decomposition of NaH at 940° F (504° C) can be observed from the figure.

Figure 9 shows the responses of two hydrogen detectors, one monitoring node 6 and the other monitoring node 23.

Figure 10 shows the hydrogen concentration at the injection node 16, the pump node 1, and the upper CCTL vessel node 27. Except for the time scale, these results are similar to those calculated by Pellow.¹²

C. Effect of Changing Flow Rate

As mentioned earlier, the CCTL test $plan^1$ includes experiments to determine hydrogen-detector response to steam injections into sodium at various flow rates. Simulations of these experiments consisted of introducing steam at 0.001 lb/sec for 70 sec at node 16 into sodium at 300, 465, 630, and 800 gpm.


Fig. 8. Transient Concentrations of Reaction Products Resulting from a Steam Injection of 0.001 lb/sec for 70 sec at Injector I4; Sodium Flow Rate of 800 gal/min at 940°F (504°C), without Cold Trapping



Fig. 9. Response of Hydrogen Detectors to a Steam Injection of 0.001 lb/sec for 70 sec at Injector I4 (See Fig. 2); Sodium Flow Rate of 800 gal/min at 940°F (504°C), without Cold Trapping

ł



Fig. 10. Transient Hydrogen Concentrations at Nodes 1, 16, and 27 Resulting from a Steam Injection of 0.001 lb/sec for 70 sec at Injector I4 (See Fig. 2); Sodium Flow Rate of 800 gal/min at 940°F (504°C), without Cold Trapping

Figure 11 shows the response of hydrogen detector No. 1 (see end of pipe 49, Fig. 2), which monitored the upper stagnant-sodium section of the steam-generator module during sodium flow rates of 300 and 800 gpm.



Fig. 11. Response of Hydrogen Detector No. 1 (See Fig. 2) at Different Sodium Flow Retes, to a Steam Injection of 0.001 lb/sec for 70 sec from Injector I4

Figures 12-15 show the response of hydrogen detector No. 3, which monitored the steam-generator outlet during sodium flow rates of 300, 465, 630, and 800 gpm, respectively.



Fig. 12. Response of Hydrogen Detector No. 3 to a Steam Injection of 0.001 lb/ sec for 70 sec at Injector I4, during Sodium Flow at 300 gpm



Fig. 13. Response of Hydrogen Detector No. 3 to a Steam Injection of 0.001 lb/ sec for 70 sec at Injector I4, during Sodium Flow at 465 gpm



Fig. 14. Response of Hydrogen Detector No. 3 to a Steam Injection of 0.001 lb/ sec for 70 sec at Injector I4, during Sodium Flow at 630 gpm



Fig. 15. Response of Hydrogen Detector No. 3 to a Steam Injection of 0.001 lb/ sec for 70 sec at Injector I4, during Sodium Flow at 800 gpm

These figures reveal that the delay between leak occurrence and detection of hydrogen concentration increases as the flow rate is decreased. If the detector is close to the leak site, as with, for example, detector number 3 in this case, the maximum transient overshoot in detector response increases when flow rate is reduced.

D. Simulation of a Tightly Coupled Loop

The flexibility of the program is demonstrated by simulating a different type of loop. In this system, the huge sodium vessel containing the steam generator is excluded. Instead, three more segments are added to the steam generator unit. A short leak of 0.015 lb/sec for a 5-sec period was injected from Injector I4 at 800 gpm and was simulated at 940°F (504°C). The results are shown in Figs. 16-20.

The oscillatory nature of the concentration changes is due to the elimination of the huge mixing volumes of the CCTL vessel, which smooth out any type of transient. A short leak, such as is simulated in this experiment, will contaminate a lump of sodium. Whenever this lump passes through a segment of the loop or near a detector, an increase in contamination is observed. After several passages, the transients die out because of the mixing process. The distance between the peaks in the figures is the transit time and is observed to be 14 sec (calculated value, 13.76 sec).



Fig. 16. Transient Hydrogen Concentration in a Tightly Coupled Loop at Pump Node 1 Resulting from a Steam Injection of 0.015 lb/sec for 5 sec into Sodium at 800 gpm and 940°F (504°C), at Injector I4



Fig. 17. Transient Hydrogen Concentrations in a Tightly Coupled Loop Resulting from a Steam Injection of 0.015 lb/sec for 5 sec at Injector I4, at 800 gpm and 940°F (504°C)



Fig. 18. Response of Hydrogen Detectors in a Tightly Coupled Loop Resulting from a Steam Injection of 0.015 lb/sec for 5 sec at Injector I4. Sodium flow is 800 gpm at 940°F (504°C).



Fig. 19. Transient Hydrogen Concentrations in a Tightly Coupled Loop Resulting from a Steam Injection of 0.015 lb/sec for 5 sec at Injector I4. Sodium flow is 800 gpm at 940°F (504°C).



Fig. 20. Transient Concentrations of Reaction Products in a Tightly Coupled Loop Resulting from a Steam Injection of 0.015 lb/sec for 5 sec at Injector I4. Sodium flow is 800 gpm at 940°F (504°C).

Similar results were obtained by Berault et al.,¹³ when a short burst of water was injected into their loop, which included mainly piping segments. The transit time was about 5 min, and 13 peaks were observed before the hydrogen diffused and mixed through system and a stable hydrogen concentration was established.

With reference to the present simulation, Fig. 16 shows the hydrogen concentration at the pump (node 1). Seven peaks occur during the first 100 sec, and the transient dies out soon thereafter.

Figure 17 compares the transient hydrogen concentrations at node 23, end of pipe 47, and the response of detector No. 3 with the transient concentration at the leaking node 16. The leak is represented by a step function 5 sec wide, after which the concentration is reduced to the background value, successive peaks appear after each transit time.

Figure 18 shows the response of hydrogen detectors No. 1 and 3. The integrating effect of the detectors compared to actual hydrogen concentration at nodes 23 and 6 is apparent.

Figure 19 shows the transient hydrogen concentration at nodes 23 and 29. Node 29 is at a "5-sec distance" from node 23. The same transient results; however, because of mixing effects, the appropriate peaks at node 29 are lower than those at segment 23.

Finally, Fig. 20 shows changes in concentration of reaction products NaH, NaOH, Na₂O, and hydrogen at node 27.

E. Effect of Cold-trap Operation

In these simulations, it was assumed that the CCTL cold trap had a static efficiency of $\beta = 0.9$, and the flow through the cold trap was 4 gal/min. Steam was introduced at Injector I4 (node 16), at a rate of 0.0001 lb/sec for 70 sec, and the simulations continued for 15 min. The results with and without cold-trap operation are shown in Figs. 21-24.

Figure 21 shows hydrogen concentrations at node 1, the pump segment. Figure 22 shows the hydrogen concentrations at node 27. Figure 23 gives the response of the hydrogen meter monitoring the steam-generator outlet. Figure 24 shows the Na₂O concentration at node 27.

These results evidence how cold-trap operation reduces impurity concentrations and is reflected in the detector readings. To obtain the new steady-state concentrations resulting from continuous cold-trap operation, the simulation would have had to be continued for about 3 hr. Due to current computer limitations, this was not considered practical. The CCTL-DYSP program has a ratio of simulation time to real time ranging from 0.2 to 0.9. For very fast rates of change in the variables and short transients, the 0.9 ratio should be taken; for slow transients and long simulation times, the 0.2 ratio can be used.



Fig 21 Effect of Cold-trap Operation on Hydrogen Concentration in the Pump Segment (Node 1)



Fig. 23. Effect of Cold-trap Operation on Hydrogen Detector Monitoring the Steam-generator Outlet

F. Effect of Different Reaction Rates

As explained previously (see Sec. III. A, C, and F), little is known about the reaction rates of the various processes occurring once the impurities enter the sodium. It is evident that simulation results cited in previous paragraphs will vary according to the assumptions made concerning the various reaction parameters. For example, the rate at which hydrogen gas leaves the sodium and enters the cover gas will be considered. It is currently assumed that the half-life of hydrogen gas-to reach equilibrium with the cover gas-is 2000 min. At this rate of hydrogen disengagement, no change in the hydrogen content in the cover gas is observed. However, if this half-life is reduced to 2 min, the



Fig. 22. Effect of Cold-trap Operation on Hydrogen Concentration in the CCTL Vessel (Node 27)



Fig. 24. Effect of Cold-trap Operation on Na₂O Concentration in the CCTL Vessel (Node 27)

hydrogen concentration in the cover gas rises sharply, as shown in Fig. 25. At least some of the uncertainties in these data are expected to be resolved by the CCTL leak-detection experiments.



Fig. 25. Change in Cover-gas Hydrogen Concentration When Hydrogendisengagement Half-life is Reduced by a Factor of 1000

G. Effect of Leak Location

The response of the CCTL experiment detector is expected to vary with the water-leak location. These changes are demonstrated in Figs. 26 and 27, which show the detector response to identical steam injections of 0.01 lb/sec for 5 sec. One injection is close to the steam-generator inlet, Injector I7; the other, Injector I1 is at the steam-generator outlet. Hydrogen detector No. 3 is monitoring the outlet from the steam-generator module. In Fig. 26, the second leak--close to the outlet--is detected first. Figure 27 shows the changes in hydrogen concentration at node 27 resulting from water injected at Injectors I1 and I7.

X. EXPERIMENTAL VERIFICATION

Recently some experimental results from the CCTL leak-detection experiment became available. On November 6, 1975, injection No. 22 took place in which 2.54 g/min of steam were injected at Injector I4. The leak duration was 57.5 sec, the sodium flow was 600 gpm, and the sodium temperature was 940°F (504° C). In Fig. 28 the experimental readings from the hydrogen



Fig. 26. Response of Hydrogen Detector No. 3 to a Steam Injection of 0.01 lb/sec for 5 sec from Two Different Injectors



Fig. 27. Transient Hydrogen Concentrations Resulting from Steam Injection of 0.01 lb/sec for 5 sec from Two Different Injectors



Fig. 28. Effect of Cold-trap Operation on Na_2O Concentration in CCTL Vessel (Node 27)

detector connected to segment 49 are superimposed on the detector response as predicted by the simulation program CCTL-DYSP. Except for random experimental noise, there is excellent agreement. Also shown are the predicted hydrogen concentrations at the end of pipe segment 40, and in the stagnant region of the heat exchanger (segment 6).

On November 7, 1975, injection No. 23 took place in which 0.98 g/min of steam was injected at Injector I4. The leak duration was 118.4 sec, the sodium flow was 300 gpm, and the sodium temperature was 940°F (504°C). In Fig. 29 the experimental readings from the hydrogen detector are superimposed on the detector response as predicted by the simulation. Small differences between the experimental and the predicted curves can be seen. These seem to be mainly due to the imperfect knowledge of the exact shape of the steam-injection curve, errors in the calculation of the delays in the sampling lines due to errors in the flowmeters, and random experimental noise, which is clearly visible on the experimental curve. In this experiment there was apparently a large calibration error in the interpretation of the detector readings. Therefore the experimental results were normalized to the steady-state result as obtained from the simulation.

XI. SUMMARY AND CONCLUSIONS

An analytical model has been developed to describe the kinetic and dynamic processes that occur when water leaks into a circulating sodium loop.

A computer code, CCTL-DYSP, solving the model equations was prepared. The distribution and the concentration of the sodium-water reaction products throughout the system was calculated, and it is shown that qualitatively the results are in agreement with similar calculations or experiments published elsewhere.^{12,13} Subsequent calculations, simulating two CCTL experiments were in good agreement with measured hydrogen concentrations (see Sec. X). However, note that experimental and theoretical information on small leaks, sodium-water interaction, and the subsequent distribution of hydrogen in a system, is scarce and of dubious validity.



Fig. 29. Changes in Cover-gas Hydrogen Concentrations When Hydrogendisengagement Half-life Is Reduced by a Factor of 1000

Most of the parameters governing hydrogen diffusion and transport throughout the system and its subsequent "evaporation" (or disengagement, if in bulk form) in the cover gas are not known. Some of the reaction parameters available, such as NaOH and HaH dissociation rates, are old data with large error limits obtained under laboratory conditions different from the actual operating conditions of the steam generator; and there is no quantitative information on how the reaction proceeds at the leak site. As a result, several assumptions had to be made and the results given in Sec. IX are dependent on these assumptions.

The contention is that the mathematical model is correct, since it is developed from basic principles. Values assumed for currently unknown parameters will be replaced with reliable experimental data, as they become available. In the meantime, the CCTL-DYSP will be used primarily to predict the response of the hydrogen and oxygen detectors during steam-generator leak-detection experiments in the CCTL. Application of the CCTL-DYSP to a CRBRP steam-generator simulation will require some changes in the routines and additional input. For example, the program should account for (1) temperature variation from segment to segment (either to be calculated or supplied as input), (2) hydrogen diffusion through the steam-generator walls, and (3) other sources and sinks of hydrogen and oxygen that may be significant. These changes will not affect the program structure; rather they will add terms to the hydrogen and oxygen sources in the appropriate routine.

APPENDIX A

Mathematical Model Used in CCTL Dynamic Simulation Program (CCTL-DYSP)

The equations and notations described in this appendix are identical to those used in CCTL-DYSP; algebraic operations are written mostly in FORTRAN symbolics.

1. An Ideal Mixing Plenum

In "ideal mixing" it is assumed the inlet stream of sodium into a segment is instantly and totally mixed with the sodium in the segment. The equations describing concentration changes of the four reaction products (i.e., C1 for NaH, C2 for NaOH, C3 for Na₂O, and C4 for hydrogen) are

$$DC1(I) = (W(I)^{*}(C1(II) - C1(I)) + CC1)/M(I) + S1(I),$$
(A.1)

$$DC2(I) = (W(I)^*(C2(II) - C2(I)) + CC2)/M(I) + S2(I),$$
(A.2)

$$DC3(I) = (W(I)^*(C3(II) - C3(I)) + CC3)/M(I) + S3(I),$$
(A.3)

and

$$DC4(I) = (W(I)^*(C4(II) - C4(I)) + CC4)/M(I) + S4(I),$$
(A.4)

where

- DC1-DC4 = time derivatives of the appropriate reaction-product concentrations,
 - I = index of the variables or number of node for which concentrations are calculated,
 - II = index number of the segment from which the main flow enters the Ith segment (usually II = I - 1),
 - M(I) = mass of the Ith segment,
 - W(I) = total flow through the Ith segment,

and CCl-CC4 account for concentration changes other than those due to the main-stream inlet and outlet for the four reaction products.

For multiple entry nodes, the following equations apply:

For node 22,

$$CC1 = WEX^*(C1(3) - C1(21)).$$
 (A.5)

For node 27,

$$CC1 = WT1*C1(50) + WT3*C1(48) + WT4*C1(46) - WDET*C1(27),$$
 (A.6)

where

$$WDET = WT1 + WT3 + WT4.$$
 (A.7)

For node 29,

$$CC1 = WCT^*(C1(43) - C1(28)).$$
 (A.8)

The S terms in Eqs. A.1-A.4 are the reaction-product sources resulting from primary or secondary reactions and are given by

$$S1(I) = KK1*QS(I)/M(I) - DNAH,$$
 (A.9)

$$S2(I) = KK2*QS(I)/M(I) - DNAOH,$$
 (A.10)

$$S_{3}(I) = KK_{3}*Q_{S}(I)/M(I) + DNAOH,$$
 (A.11)

 and

$$S4(I) = KK4*QS(I)/M(I) + (DNAH + DNAOH)*0.5 - WH/M(I),$$
 (A.12)

where

QS(I) = leak rate at the Ith node,

- WH = rate of hydrogen escape from the segment into the cover-gas plenum,
- $DNAH = RR1*C1(I), \qquad (A.13)$

$$DNAOH = R3*C2(I),$$
 (A.14)

RR1 = NaH dissociation rate,

$$RR1 = 0.597*EXP(-3833/TK)*((PDIS - PH)/PDIS)^{2}$$
(A.15)

TK = Kelvin temperature of sodium,

$$TK = (TEMP - 32)/1.8 + 273,$$
(A.16)

TEMP = sodium temperature (in $^{\circ}F$), which is an input value,

PDIS = NaH dissociation pressure,

PH = hydrogen partial pressure,

and

R3 = NaOH dissociation rate, which is an input value.

Finally, the actual values of the reaction-product concentrations are obtained by integrating the derivatives in Eqs. A.1-A.4 by an integration routine. Presently a simple Euler formula is used, but any integration procedure can be chosen.

2. Node with Cover Gas

The term WH in Eq. A.12 is given by

$$WH = R1^*(C4(I) - CHNA)$$
 for CHNA > C4(I), (A.17)

where

R1 = hydrogen-gas disengagement constant,

CHNA = hydrogen concentration in sodium that would be achieved under equilibrium conditions according to Sieverts' constant,

 $CHNA = KS^*SQRT(PH), \qquad (A.18)$

and

KS = Sieverts' constant, KS = $EXP(1.9733 - 276.77/TK)*453.6/2.0116*10^{-6}$. (A.19)

The partial hydrogen pressure PH in the cover gas is calculated from the ideal gas laws, and is given by

$$DPH = (WHPU + WHCT)*554*TPLEN/VPLEN, \qquad (A.20)$$

where

WHPU = hydrogen gas escaping through the pump, WHCT = hydrogen gas escaping through the CCTL vessel, TPLEN = absolute temperature in the cover gas, TPLEN = TEMP + 460,

and

VPLEN = total volume of gas plenum, including the CCTL vessel, the expansion tank, and the pump tank.

Finally, DPH is integrated to obtain PH.

3. Pipe Node and Generating Delay Functions

A pipe in the system generates a time lag or holds up an event occurring at the pipe inlet for a period equivalent to the passage time through the pipe.

A time lag for a specified event is generated by storing the appropriate concentrations at the pipe-inlet node along with appropriate time values. Each pipe segment is allocated 100 memory locations. Pipe-inlet values are stored initially at constant time intervals. When the simulation starts, these values are stored whenever a change larger than PDEL in the pipe-inlet variable oc-curs; PDEL is usually 0.5 or 1%. When the outlet variable of a pipe segment is required, the lag time τ is first calculated by

$$\tau = M(I)/W(I).$$
 (A.21)

Then the value of the variable is calculated by linear interpolation of the two closest variables available at time t $-\tau$ in a pipe function.

The secondary reactions in the pipe are accounted for by the following equations. Assuming FX1, FX2, FX3, and FX4 are the pipe-outlet variables at time $t - \tau$, the true pipe-outlet concentrations are given by

$$C1(I) = FX1 + S1(I)^*\tau,$$
 (A.22)

$$C2(I) = FX2 + S2(I)^*\tau,$$
 (A.23)

$$C3(I) = FX3 + S3(I)^*\tau,$$
 (A.24)

$$C4(I) = FX4 + S4(I)^*\tau,$$
 (A.25)

where

$$S1(I) = -RR1*FX1,$$
 (A.26)

S2(I) = -R3*FX2, (A.27)

$$S3(I) = -S2(I),$$
 (A.28)

and

$$S4(I) = -(S1(I) + S2(I)*0.5.$$
 (A.29)

4. Cold Trap

The cold trap causes reaction products to precipitate at a rate

$$W42 = BETA^*(C1(42) - C1SAT),$$
(A.30)

 and

$$W420 = BETA^*(C3(42) - C3SAT),$$
 (A.31)

where

W42 = precipitation rate of NaH,

W420 = precipitation rate of Na_2O ,

BETA = dynamic cold-trap efficiency,

C1SAT = saturation concentration of NaH,

$$C1SAT = 453.6*10^{-6}/23.9983*EXP(13.93 - 6631.4/TCLT),$$
 (A.32)

$$C3SAT = saturation concentration of Na_2O$$
,

$$C3SAT = 453.6*10^{-6}/61.98*EXP(16.131 - 6493.3/TCLT),$$
(A.33)

where

TCLT = absolute cold-trap temperatureTCLT = (TCLT - 32)/1.8 + 273(A.34)

5. Detectors

The derivative of a hydrogen-detector response is given by

$$DPP = (CD1 + CD4 - CDET(N))/TDLE(N), \qquad (A.35)$$

where

- TDLE(N) = diffusion delay time of Nth hydrogen detector,
- CDET(N) = response of Nth detector obtained by integrating DPP or the detector internal hydrogen concentration,

$$CD1 = (FX1 + SD1*TAU)*1.0083*10^{6}/453.6,$$
 (A.36)

and

$$CD4 = (FX4 + SD4*TAU)*2.0166*10^{6}/453.6.$$
 (A.37)

FX1 and FX4 are hydride and hydrogen concentrations, respectively, at the outside of detector membrane, and are equal to the monitored segment concentration at time TIME - TAU, where TAU is given by

$$TAU = M(N1)/W(N1) + TLAG(N).$$
 (A.38)

In Eq. A.38, M(N1) and W(N1) are the mass and the flow rate of the monitoring bypass pipe segment, and TLAG is the time lag of the Nth detector. The hydrogen-detector response in ppm is obtained by integrating Eq. A.35. The oxygen-detector response is calculated from

$$DPP = (CD3 - CDET(N))/TDLE(N), \qquad (A.39)$$

where

$$CD3 = (FX3 + SD3^{*}TAU)^{*16.0^{*}10^{6}/453.6}$$
(A.40)

and

$$SD3 = R3*FX2.$$
 (A.41)

The oxygen-meter response is obtained by integrating Eq. A.39. The readout of the hydrogen meter in the cover gas is proportional to the hydrogen partial pressure. The readout is converted to ppm by volume using the relation

$$CD4 = PH^{10^6}/(PH + PA),$$
 (A.42)

where

PH = hydrogen partial pressure

and

PA = argon-cover-gas partial pressure.

The detector response is calculated by integrating

$$DPP = (CD4 - CDET(N))/TDLE(N), \qquad (A.43)$$

where CDET(N) is the detector response, and TDLE(N) is the delay time of the Nth detector.

Description of CCTL-DYSP

A simplified schematic of the simulation program is shown in Fig. B.1. The program 1s written in FORTRAN in a modular form. It has five calculating



Fig. B 1. Simplified Schematic Flowchart of CCTL-DYSP

subroutines, a coordinating main program, two service subroutines for printing and plotting results, and a small integrating routine.

The main coordinating program first calls the INIT routine in which data are read in, initial values are calculated and printed, and the pipe initial function is set up. The program then proceeds to the dynamic phase by increasing time by a time step, and increasing the time-step counter by 1.

The first subroutine called in the dynamic section is SOURCE. This routine calculates the source of reaction products resulting from any type of chemical reaction at each loop segment. Equations A.5-A.19 are solved.

The second routine called is INTEGR, which computes the derivatives of all reaction-product concentrations in the loop segments and pipe outlets. This routine has access to the PIPE subroutine to compute pipeoutlet concentrations, and to the INTGI routine, which performs the actual integration.

The main program then accesses the DETECT subroutine, which computes the appropriate detector responses.

After the variables for a time step have been calculated by appropriate integration of the differential equations, the program updates the inlet variables for the pipe segments by calling PIPE. The program then enters the PRIT routine, and, if requested, some data such as detector responses and concentrations at some of the nodes are printed. Every TPR seconds--as determined by the input parameter--a complete "map" of the system is printed, which includes derivatives, sources, and actual concentration of the four reaction products at each segment and pipe outlet. The SPLOT routine is entered next, and user-selected data are stored in a specific file for later plotting.

Finally, the program checks the time; if it is less than the predeter mined length of simulation, a time-step calculation is repeated. If the time is equal to the final simulation time, the program terminates by printing a final "map" of the system and print-plotting the results previously stored in a file. The listing of the program is given in Appendix C, and the input data are described in Appendix D.

APPENDIX C

Listing of CCTL-DYSP

CCTL_FORT PRESENT DATE 8/11/76 DSK203 5 [------------C 10 C С 15 C CCTL-DYSP: A DYNAMIC SIMULATIUN PROGRAM TU CALCULATE HYDRUGEN С AND OXYGEN CONCENTRATION IN WATER TO SODIUM LEAK EXPERIMENT IN 20 C С 25 C THE CORE COMPONENT TEST LOOP. С С 30 C 35 C PRUGRAM CAPACITY: C C 40 C 50 SEGMENTS С 45 C DETECTORS 7 С 50 C REACTION PRODUCTS CONCENTRATIONS 4 CUMBINED COVER GAS PLENUM С 55 C 1 60 C COLD TRAP С 1 65 C С - C 70 C------75 ...#C 90 C#........ 95 C#. .#C 100 C#. A - CRUSS SECTION AREA OF SEGMENT (FT**2) .#C 105 C#. ABSC - THE HEADING TO BE PRINTED ALONG THE ABSCISAE OF .#C **.**#C 110 C#. GRAPHIC OUTPUT 115 C#. BETA - RATE AT WHICH NAH IS REMOVED IN THE CULD TRAP .#C 120 C#. C1 - CUNCENTRATION OF NAH (MOL/LB) .#C 125 C#. CISAT - SATURATION CONCENTRATION UF NAH AT COLD TRAP TEMPERATURES.#C 130 C#. C2 - CONCENTRATION UF NACH (MUL/LB) .#C **.**#C 135 C#. C3 - CONCENTRATION OF NA20 (MOL/LB) 140 C#, C4 - CONCENTRATION OF H2 (MOL/LB) **.**#C **.**#C 145 C#. CDET - DETECTOR READING IN PPM 150 C#. FIGTTL - TITLE GIVE TO A FIGURE DRAWN BY THA CALCOMP PLUTTER •#C 155 C#. FINTIM - SIMULATION TIME FOR THIS RUN IN (SEC) .#C 160 C#. IC - NODE NUMBERS FOR WHICH CINCENTRATIONS TO BE PLOTIED **"**#C 165 C#. ICT - NUDE NUMBERS FOR WHICH PPM CONC OF H2 IS PRINTED PER STEP .#C 170 C#. IQ - NUMBER OF NODE AT WHICH LEAKAGE MIGHT OCCURE .#C 175 C#. JPL - PLOTTING COUNTER **.**#C **.**#C 180 C#. JPR - PRINTING CUUNTER .#C 185 C#. JT - TIME STEP COUNTER .#C 190 C#. K1 - FRACTION OF H20 LEAK TO: NA+H20=NAOH+1/2H2(G) 195 C#. K2 - FRACTION OF H20 LEAK TU: 2NA+H20=NAOH+NAH .#C 200 C#. K3 - FRACTION OF H2U LEAK TU: 3NA +H2U=2NAH+NA2O .#C 205 C#. K4 - FRACTIUN UF H20 LEAK TU: 2NA+H20=NA20+H2 .#C 206 C#. KH - IF 1 WATER LEAK, IF 2 HYDRUGEN LEAK. 210 C#. L - LENGTH UF SEGMENT (FT) .#C 215 C#. LG - SEGMENT IDENTIFICATION NUMBER: 0 NO SEGMENT .#C 1 PLENUM MIXED SEGMENT .#C 250 C#* **.**#C 225 C#. 2 PIPE SEGMENT 230 C#. 3 PLENUM MIXING WITH COVER GA.#C 5 PLENUM WITH CUVER AND MULTE_#C 235 C#. 240 C#. M - MASS OF SUDIUM IN SEGMENT **.**#C .#C 245 C#. NAME - NAME OF APPROPRIATE VECTUR TO BE PLOITED 250 C#. NGRAF - NU. UF CURVES TO BE PRINTPLUTTED OR PLOTTED PER FIG. .#C 255 C#. NUDE - NUMBER OF NODE TO WHICH DETECTUR IS CONNECTED .#C 260 C#. NTYPE - TYPE OF DETECTOR USED MONITORING AT SEGMENT 'NODE' .#C

CCTL.FURT

.#C 265 C#, NUDET - NUMBER UF DETECTORS IN THE SYSTEM 270 C#. PA - ARGUN PARTIAL PRESSURE IN COVER GAS .#C .#C 275 C#. PDIS - NAH DISSUCIATION PRESSURE 280 C#. PDEL - MAXIMUM PERMITED CHANGE IN NODE 23 FUR PIPE UPDATA .#C 285 C#. PH - HYDRUGEN PARIIAL PRESSURE IN CUVER GAS (MM-HG) .#C 290 C#, PRT1 - IF TRUE INITIAL PIPE FUNCTION DISTRIBUTION WILL BE _#C .#C 295 C#. PRINTED 300 C#. PRT2 - RESERVED .#C 305 C#. PRT3 - KESERVED .#C .#C 310 C#. PRT4 - RESERVED 315 C#. PRT5 - IF TRUE A CALCUMP 580 PLUT UF THE PREDETERMINED VARI-.#C .#C ABLES WILL BE PREPARED 320 C#. 322 C#. PTDL - MAXIMUM PERMITED TIME INTERVAL FUR PIPE UPDATE .#C **.**#C 325 C#. Q - H20 LEAKAGE IN THE I-TH NODE (LUS/SEC) 330 C#. R1 - RATE OF H2 DISENGAGEMENT FROM LIQUID NA TO COVER GAS (SEC-1).#C .#C 335 C#. R2 - RATE OF NAH DISSUCIACION NAH=NA+H (SEC-1*MM-HG-2) **.**#C 340 C#, R3 - RATE OF NACH DISSOCIATION NAUH+NA=NA2O+H (SEC-1) **.**#C 345 C#. S1 - SOURCE OF NAH (MUL/SEC) **.**#C 350 C#. S2 - SOURCE OF NAUH (MOL/SEC) 355 C#. S3 - SOURCE OF NA2O (MOL/SEC) .#C **.**#C 360 C#. S4 - SOURCE OF H2 (MUL/SEC) 365 C#. TQ - TIME AT WHICH LEAKAGE AT I-TH NODE STARTS (SEC) .#C 370 C#. TX - TIME AT WHICH LEAKAGE AT I-TH NODE TERMINATES (SEC) **.**#C 375 C#. TCLT - COLD TRAP TEMPERATURE (DEG F OR K) .#C 380 C#. TDLE - DIFFUSION TIME CUNSTANT FOR DET. NICKEL MEMBRANE (SEC) **.**#C **.**#C 385 C#. TEMP - SUDIUM TEMPERATURE (DEG F) 390 C#. TIME - CURENT SIMULATION TIME (SEC) .#C 395 C#. TLAG - TIME LAG BETWEEN DETECTOR SAMP.LINE INLET AND DETECTOR (SE.#C **.**#C 400 C*. TMM - TOTAL SODIUM MASS IN CCTL (L8S) **.**#C 405 C*. TMT - TOTAL CUOLANT TRANSIT TIME (SEC) **.**#C 410 C#. TPL - PLOTING INTERVAL (SEC) 415 C#. TPR - PRINTING INTERVAL (SEC) .#C 420 C#. WCT - FLOW THROUGH THE COLD TRAP IN (GPM) .#C **.**#C 425 C*. WS - TUTAL SUDIUM FLOW IN CCTL (GPM) **.**#C 430 C#, WT1 - FLOW TO DETECTOR # 1 (LBS/SEC) .#C 435 C#. WT2 - FLOW TO DETECTUR # 2 (LBS/SEC) ,#C 440 C#. WT3 - FLUW TO DETECTOR # 3 (LBS/SEC) **.**#C 445 C#. WT4 - FLOW TO DETECTOR # 4 (LBS/SEC)#C 450 C#...... 460 COMMON /BLK/ L,A,M,C1,C2,C3,C4,LG,WS,WCT,WT1,WT2,WT3,WT4,WEX,TEMP, 465 470 C FINTIM, RONA, DTMIN, DTMAX, S1, S2, S3, S4, JT, KS, TPR, IQ, ICT, W, JCT, C WR,WA,WX,WB,WC,WD,WE,Q,TQ,TX,QS,PDIS,PH,PA,K1,K2,K3,K4,R1,R2,R3, 475 480 C WHCT, WHPU, TPLEN, VPLEN, IC, TPL, CHNA, RR1, QX, QXT, QHT, C1SAT, BETA, C ALFA, TMM, NPICT, NGRAF, NVECT, NAME, IPI, NUDET, NUDE, NTYPE, 485 C TLAG, CDET, TDLE, C3SAT, PDEL, FIGTTL, PTDL, KH 490 495 COMMON /LUG/ TITLE, PRI1, PRT2, PRT3, PRT4, PRT5 COMMON /DUB/ TIME, DELT, DC1, DC2, UC3, DC4, ABSC 500 REAL * 4 L(50), A(50), M(50), C1(50), C2(50), C3(50), C4(50), W(50)505 REAL *4 S1(50), S2(50), S3(50), S4(50), Q(8), TQ(8), TX(8), QS(50) 510 515 REAL+4 K1,K2,K3,K4,KS,TITLE(18),TLAG(7),CDET(7),TDLE(7) REAL*8 DC1(50),DC2(50),DC3(50),DC4(50),TIME,DELT,ABSC(4,10) 520

```
525
           LOGICAL PRT1, PRT2, PRT3, PRT4, PRT5
530
           DIMENSION LG(50), IQ(8), IC(8), ICT(8), NGRAF(10), NVECT(10,5),
535
          C NAME(10,15), IPI(50), NODE(7), NTYPE(7), FIGTTL(15,10)
540
545
           CALL INIT
550
           LV=1
555
           QXT=0.
           C40LD=C4(23)
560
565
           TOLD=0.
570
           GOTO 20
           START TIME DEPENDENT CALCULATIONS
575 C****
580
      10
           TIME=TIME+DELT
585
           JT = JT + 1
590
           CALL SOURCE
           CALL INTEGR
595
600
           CALL DETECT
605 C**** UPDATE PIPE FUNCTIONS IF CHANGE > PDEL UR ELAPSED TIME MORE THEN .
610 C**** 0.5 SECUNDS
615
           TIM=TIME
           CHNG=(C40LD-C4(23))/C40LD
620
           CHTM=TIM-TOLD
625
630
           IF (ABS(CHNG).LT.PDEL.AND.CHTM.LT.PTDL) GOTO 20
635
           TULD=TIM
           C40LD=C4(23)
640
645
           DEL=DELT
650
           CALL PIPE(TIM, DEL, 0.0, 1, C1(1), C2(1), C3(1), C4(1))
           CALL PIPE(TIM, DEL, 0, 0, 2, C1(3), C2(3), C3(3), C4(3))
655
           CALL PIPE(TIM, DEL, 0.0, 3, C1(23), C2(23), C3(23), C4(23))
660
665
           CALL PIPE(TIM, DEL, 0, 0, 4, C1(27), C2(27), C3(27), C4(27))
670
           CALL PIPE(TIM, DEL, 0, 0, 5, C1(29), C2(29), C3(29), C4(29))
675
           CALL PIPE(TIM, DEL, 0, 0, 6, C1(6), C2(6), C3(6), C4(6))
680
           CALL PIPE(TIM, DEL, 0, 0, 7, C1(25), C2(25), C3(25), C4(25))
685
           CALL PIPE(TIM, DEL, 0.0, 8, C1(42), C2(42), C3(42), C4(42))
690
           CALL PIPE(TIM, DEL, 0.0, 10, RR1, PH, CHNA, 0.0)
695 C**** PERFORM TUTAL HYDROGEN BALANCE CALCULATIONS FOR THIS TIME STEP
700
       20 QX=0.
           GHT=0.
705
710
           DO 92 I=1,50
           IF(LG(I).EQ.0) GUTO 92
715
720
           QHT=QHT+(0.5*C1(I)+0.5*C2(I)+C4(I))*M(I)
725
           QX=QX+QS(I)
       92 CONTINUE
730
735
           QXT=QXT+QX*DELT
           QHT=QHT+PH*VPLEN/(TPLEN*554.0)
740
745
           ALFA=(0.5*C1(ICT(1))+C4(ICT(1)))*TMM/QHT
750
           CALL SPLOT(LV)
755
           CALL PRIT(LV)
           TIM=TIME
760
765
           LV=2
           IF (FINTIM-TIM.GT.DELT/2) GOTO 10
770
           CALL PRIT(3)
775
780
           CALL SPLUT(3)
785
           STOP
```

790 END 795 -C 800 C----805 C C 810 C С SUBROUTINE INIT С 815 C THIS SUBROUTINE INITIALIZES THE PROGRAM, READS INPUT DATA 820 C AND SUPPLIES DEFAULT VALUES TO DATA NOT IN INPUT STREAM C С 825 C • C 830 C-----835 840 SUBROUTINE INIT COMMON /BLK/ L,A,M,C1,C2,C3,C4,LG,WS,WCT,WT1,WT2,WT3,WT4,WEX,TEMP, 845 850 C FINTIM, RUNA, DTMIN, DTMAX, S1, S2, S3, S4, JT, KS, TPR, IQ, ICT, W, JCT, 855 WR,WA,WX,WB,WC,WD,WE,Q,TQ,TX,QS,PDIS,PH,PA,K1,K2,K3,K4,R1,R2,R3, C 860 C WHCT, WHPU, TPLEN, VPLEN, IC, TPL, CHNA, RR1, QX, QXT, QHT, C1SAT, BETA, C ALFA, TMM, NPICT, NGRAF, NVECT, NAME, IPI, NUDET, NUDE, NTYPE, 865 870 C TLAG, CDET, TDLE, C3SAT, PDEL, FIGTTL, PTDL, KH CUMMON /LOG/ TITLE, PRT1, PRT2, PRT3, PRT4, PRT5 875 COMMON /DUB/ TIME, DELT, DC1, DC2, DC3, DC4, ABSC 880 $REAL \pm 4$ L(50), A(50), M(50), C1(50), C2(50), C3(50), C4(50), W(50) 885 890 REAL*4 S1(50),S2(50),S3(50),S4(50),Q(8),TU(8),TX(8),QS(50) REAL*4 K1,K2,K3,K4,KS,TITLE(18),TLAG(7),CDET(7),TDLE(7) 895 REAL*8 DC1(50), DC2(50), DC3(50), DC4(50), TIME, DELT, ABSC(4,10) 900 LOGICAL PRT1, PR12, PRT3, PRT4, PRT5 905 910 REAL *4 MOL DIMENSION LG(50), IQ(8), IC(8), IC(8), NGRAF(10), NVECT(10,5), 915 920 C NAME(10,15), IPI(50), NODE(7), NTYPE(7), FIGTTL(15,10) 925 DIMENSION ADAT(20) DATA PI/3.1416/,CFPG/.13368981/,ADA/'9999'/ 930 935 C 1 READ 180, ADAT 940 945 PRINT 190, ADAT 950 IF (ADAT(1).NE.ADA) GOTO 1 955 REWIND 5 NAMELIST /INLST/ L,LG,A,C1,C2,C3,C4,Q,TQ,TX,IQ,IC,ICT 960 965 C /PARM/ TEMP,WS,WCT,WT1,WT2,PH,PA,K1,K2,K3,K4,R1,R3,BETA,C1SAT, 970 C WT3,WT4,WEX,FINTIM,DELT,DTMIN,DTMAX,TPR,VPLEN,TPL,JCT, C PRT1, PRT2, PRT3, PRT4, PRT5, BETA, TCLT, PUEL, PTDL, KH 975 980 C /DTCTR/ NUDET, NODE, NTYPE, TDLE, TLAG 985 READ 200, TITLE 990 READ (5, INLST) 995 READ (5, PARM) READ (5,DTCTR) 1000 1005 **READ 210** 1010 READ 170, NPICT 1015 READ 170, NGRAF DU 3 N=1,NPICT 1020 NN=NGRAF(N) 1025 READ 170, (NVECT(N, I), I=1, NN) 1030 READ 220, ((NAME(N, (I-1)*3+J), J=1,3), I=1, NN) 1035 1040 READ 230, (ABSC(I,N), I=1,4) READ 200, (FIGTTL(I,N), I=1,15) 1045 1050 **3 CONTINUE**



•

1055		RONA=59,566-TEMP*(7,9504E-3+TEMP*(2,872E-7-TEMP*6,035E-11))
1060		MOL=453,6/18,02
1065		Q = 0
1070		QXT=0.
1075		WS=WS*CFPG*RUNA/60.
1080		WCT=WCT+CFPG+RONA/60.
1085		WT1=WT1+CFPG*RONA/60.
1090		WIZ=WIZ*CFPG*RONA/60.
1095		WT3=WT3*CFPG*RONA/60.
1100		WT4=WT4+CFPG+RONA/60.
1105		WEX=WEX*CFPG*RONA/60.
1110		WAINS-WEX
1115		WX=WA-W11-W72
1120		WB=WX+WFX
1125		WC=WB-WT3
1130		
1135		WF=WD+W11+W12+W13+W14
1140		WR=wE+wCT
1145		
1150		D() 5)=1.8
1155	5	$Q(I) = Q(1) \times MOL$
1160	-	$C_1(1) = C_1(1) + 453 - 6/23 - 9986$
1165		C2(1)=C2(1)*453.6/39.9983
1170		$C_3(1) = C_3(1) + 453.6/61.98$
1175		C4(1)=C4(1)*453.6/2.0166
1180		TCLT=(TCLT-32.0)/1.8+273.0
1185		C1SAT=453.6E-6/23.9983*EXP(13.97-6631.4/TCLT)
1190		C3SAT=453.6E=6/61.98*EXP(16.131=6493.3/TCLT)
1195		IF(C1(1).EQ.0.0) C1(1)=C1SAT
1200		IF(C3(1).EQ.0.0) C3(1)=C3SAT
1205		DU 10 I=1,50
1210		IPI(I)=0
1215		C1(I)=C1(1)
1220		C2(I)=C2(I)
1225		C3(I)=C3(1)
1230		C4(I)=C4(1)
1235		IF(LG(I).NE.0) GOTO 9
1240		C3(I)=0.
1245		C4(I)=0.
1250		C1(1)=0.
1255		C2(1)=0.
1260	9	W(I)=0.
1265		S1(I)=0.
1270		\$2(1)=0.
1275		\$3(1)=0.
1280		S4(I)=0.
1285		US(I)=0 .
1290		M(I)=L(I)*A(I)*RUNA
1295		FMM=TMM+M(I)
1300		DC1(I)=0.
1305		DC2(I)=0.
1310		DC3(I)=0.
1315		DC4(I)=0.

```
1320
        10 CONTINUE
1325 C**** INITIALIZE DETECTOR READING
1330
            DO 11 N=1,NUDET
1335
            NTP=NTYPE(N)
1340
            GUTO (12,13,14), NTP
1345
         12 CDET(N)=(0.5*C1(1)+C4(1))*2,0100E+6/453,3
1350
            GOTO 11
        13 CDET(N)=C3(1)*10.0E+0/453.3
1355
1360
            GOTO 11
        14 CUET(N)=PH*1.0E+6/(PA+PH)
1365
1370
         11 CONTINUE
1375
            M(46) = M(46) + M(45)
1380
            M(48) = M(48) + M(47)
1385
            M(50) = M(50) + M(49)
1390
            TM=0.
1395
            DU 15 I=1,30
1400
         15 TM=TM+M(I)
1405
            TM=TM-M(6)
1410
            TMT=TM/WS
            1P=0
1415
1420
            CALL PIPE(TIME, DELT, 0., IP, C1(1), C2(1), C3(1), C4(1))
1425
            TK=(TEMP=32.)/1.8+273.
1430
            TPLEN=TEMP+460.
1435
            KS=EXP(1.9733-276.77/1K)*453.6/2.0116*1.E=6
1440
            PDIS=EXP(26.71-14046.0/TK)
1445
            R2=0.597*EXP(-3833/TK)
1450 C
1455 C**** CALCULATE TUTAL FLOW THROUGH EACH SEGMENT
1460
            W(1) = WR
1465
            W(2)=WS
1470
            W(3) = WS
1475
            w(4)=wA
1480
            W(5)=WA
1485
             W(0)=W11+W12
1490
             W(7)=WA
1495
             DO 20 I=8,21
1500
        50 M(I)=MX
1505
             W(22)=WB
1510
             W(23) = WB
1515
             W(24)=WC
1520
             W(25)=WC
1525
             W(26)=WD
1530
             W(27)=WE
             W(28)=WE
1535
1540
            W(29)=WR
1545
            W(30) = WR
1550
            W(41) = WCT
1555
            W(42)=WCT
1560
            w(43)=WCT
1565
            W(45)=WT4
1570
            W(46)=WT4
1575
            w(47)=wT3
1580
            W(48) = WT3
```

1585 W(49) = WT11590 W(50) = WT11595 C**** SET APPROPRIATE PIPE FUNCTION NUMBERS TU PIPE SEGMENTS IPI(2)=11600 IPI(4)=21605 IPI(24) = 31610 1615 IP1(47)=31620 IPI(48) = 31625 IPI(28) = 41630 IPI(30)=51635 IPI(41) = 7IPI(45) = 71640 1645 IPI(46) = 7IPI(49) = 61650 IPI(50)=61655 IPI(43) = 81660 1665 BETA=BETA * W (42) / M (42) CALL SOURCE 1670 1675 CALL PIPE(TIME, DELT, 0.0, 10, RR1, PH, CHNA, 0.0) 1680 C 1685 C**** PRINT INITIAL DATA PRINT 300, TITLE 1690 PRINT 100 1695 PRINT 110, IQ,Q,TQ,TX 1700 YK1=K2+2.*K3 1705 YK2=K1+K2 1710 YK3=K3+K4 1715 1720 YK4=0.5*K1+K4 1725 PRINT 150,K1,K2,K3,K4,YK1,YK2,YK3,YK4 1730 PRINT 120, PDIS 1735 PRINT 130, TEMP, TK, RONA, TMM, VPLEN, BETA, C1SAT, C3SAT, TMT, TCLT, KS 1740 PRINT 140, WS,WCT,WT1,WT2,WT3,WT4,WEX,WA,WX,WB,WC,WD,WE,WR 1745 PRINT 160,(N,NTYPE(N),NUDE(N),TLAG(N),TDLE(N),N=1,NUDET) 1750 99 RETURN FORMAT(1H , ' LEAKAGE DATA FUR THIS CASE ARE:') 1755 100 110 FORMAT(1H0, 'FOR NUDE SEGMENT # 1760 ',8I12/ ' THE LEAKAGE IN MOL/SEC IS',8E12.4/ 1765 С ' THE LEAK STARTS AT TIME -',8F12.2/ 1770 C. 1775 ' THE LEAK IS TERMINATED AT',8F12.2/) С 1780 120 FORMAT('OTHE NAH DISSUCIATION PRESSURE IN MM-HG IS', F12.3) 130 FORMAT(' SODIUM TEMPERATURE IN (DEG-F)IS 1785 ',F12.2/ I SODIUM TEMPERATURE IN (DEG-K) IS 1790 С ',F12.2/ SODIUM DENSITY IN (LBS/CUF) IS 1795 С . ',F12.2/ ' TOTAL WEIGHT OF SODIUM IN THE SYSTEM (LB)', F12.2/ С 1800 ' COVER GAS PLENUM VULUME (CUF) ',F12.2/ С 1805 ',E12.4/ COLD TRAP DYNAMIC EFFICIENCY (1/SEC) IS 1810 С ' NAH SATURATION CONC. AT COLD TRAP(MOL/LB)', E12.4/ С 1815 С ' NA2U SATURATION CNC. AT COLD TRAP(MOL/LB)',E12.4/ 1820 1825 С ' TOTAL TRANSIT TIME IN CCTL (SEC) IS ',F12.2/ COLD TRAP TEMPERATURE IN (DEG-K) IS ',F12.2/ 1830 С 1835 С ' SIEVERTS CONSTANT IN (MOL/(LB*TORR**=2)) ',E12.4) 1840 140 FORMAT('OTOTAL SODIUM FLOW IN (LBS/SEC) IS ', F12.4, 1845 C/30X, 'WCT', 9X, F12.4/30X, 'WT1', 9X, F12.4/30X, 'WT2', 9X, F12.4/

1850 C 30X, 'WT3', 9X, F12.4/30X, 'WT4', 9X, F12.4/30X, 'WEX', 9X, F12.4/ 1855 C 30X, WA ', 9X, F12.4/30X, WX ', 9X, F12.4/30X, WB ', 9X, F12.4/ C 30X, WC ', 9X, F12.4/30X, WD ', 9X, F12.4/30X, WE ', 9X, F12.4/ 1860 30X, WR 1, 9X, F12, 4//) 1865 C 1870 170 FORMAT(10(12,1X)) 1875 150 FORMAT(1X, F4.2, ' UF THE LEAK GOES TO NA+H2O=NA0H+1/2H2(G)'/ 1X, F4.2, ' OF THE LEAK GOES TO 1880 2NA+H2O=NAOH+NAH'/ C 1X, F4.2, ' UF THE LEAK GUES TU 1885 C 4NA+H20=2NAH+NA20 / 1X,F4.2, ' OF THE LEAK GOES TO 1890 С 2NA+H20=NA20+H2!/ С 1X,F4.2,' MOL UF THE LEAK IS TRANSFORMED TU NAH'/ 1895 1900 С 1X,F4.2,' MUL UF THE LEAK IS TRANSFORMED TO NAUH'/ 1X,F4.2, ' MOL OF THE LEAK IS TRANSFORMED TO NA20'/ 1905 С 1X,F4.2,' MOL OF THE LEAK IS TRANSFORMED TO H2(G)') 1910 С 160 FORMAT(1H0, ' DETECTOR NO ', I1, ' OF TYPE ', I1, ' IS CONECTED', 1915 1920 C ' TO NODE ', I2, ' HAS A LAG OF ', F5.2, 'SEC AND A DELAY OF', 1925 C F5.2, 'SEC') 1930 180 FURMAT(20A4) 1935 190 FORMAT(10X,20A4) 1940 200 FURMAT(18A4) 1945 210 FORMAT(80x) 1950 220 FORMAT(5(3A4,1X)) 1955 230 FORMAT(4A8) 1960 300 FORMAT('1',20('*'),18A4,20('*')//) 1965 END 1970 -C 1980 C С С 1985 C SUBROUTINE SOURCE. 1990 C IN THIS SUBROUTINE SOURCES AND SINKS OF THE REACTION PRODUCTS С 1995 C С ARE CALCULATED С 2000 C 2005 C-------C 2010 2015 SUBROUTINE SOURCE 2020 COMMON /BLK/ L,A,M,C1,C2,C3,C4,LG,WS,WCT,WT1,WT2,WT3,WT4,WEX,TEMP, 2025 C FINTIM, RUNA, DTMIN, DTMAX, S1, S2, S3, S4, J1, KS, TPR, IQ, ICT, W, JCT, 2030 C WR,WA,WX,WB,WC,WD,WE,Q,TQ,TX,QS,PDIS,PH,PA,K1,K2,K3,K4,R1,R2,R3, 2035 C WHCT, WHPU, TPLEN, VPLEN, IC, TPL, CHNA, RR1, WX, WXT, WHT, C1SAT, BETA, 2040 C ALFA, TMM, NPICT, NGRAF, NVECT, NAME, IPI, NUDET, NODE, NTYPE, 2045 C TLAG, CDET, TDLE, C3SAT, PDEL, FIGTTL, PTDL, KH 2050 COMMON /LOG/ TITLE, PRT1, PRT2, PRT3, PRT4, PR15 COMMON /DUB/ TIME, DELT, DC1, DC2, DC3, DC4, ABSC 2055 2060 REAL*4 L(50),A(50),M(50),C1(50),C2(50),C3(50),C4(50),W(50) 2065 REAL*4 S1(50),S2(50),S3(50),S4(50),Q(8),TQ(8),TX(8),QS(50) REAL*4 K1,K2,K3,K4,KS,TITLE(18),TLAG(7),CDET(7),TDLE(7) 2070 DIMENSIUN LG(50), IQ(8), IC(8), ICT(8), NGRAF(10), NVECT(10,5), 2075 2080 C NAME(10,15), IPI(50), NODE(7), NTYPE(7), FIGTTL(15,10) 2085 REAL *4 KK1, KK2, KK3, KK4 2090 REAL*8 DC1(50), DC2(50), DC3(50), DC4(50), TIME, DELT, ABSC(4,10) 2095 LOGICAL PRT1, PRT2, PRT3, PRT4, PRT5 2100 C 2105 C**** CALCULATE REACTION RATES 2106 GOTO (1,3),KH

1 KK1=K2+2*K3

2110

```
2115
            KK2=K1+K2
2120
            KK3=K3+K4
2125
            KK4=0.5*K1+K4
2126
            GUTO 4
          3 KK1=2*K1
2127
2128
            KK2=0
2129
            KK3=0
            KK4=1.-K1
2130
          4 RR1=((PDIS+PH)/PDIS)*ABS((PDIS-PH)/PDIS)*R2
2134
            CHNA=KS*SQRT(PH)
2135
2140 C
2145 C**** DETERMINE LEAKAGE SOURCES
2150
            DU 2 I=1,8
2155
            I2=IQ(I)
            QS(I2)=0.0
2160
2165
            IF(TIME.GE.TQ(I).AND.TIME.LE.TX(I)) QS(I2)=Q(I)
2170
         2
            CONTINUE
2175 C
2180 C**** CALCULATE SUURCES IN MOL/SEC
2185
            DO 10 I=1,50
2190
            IF(LG(I).EQ.0.OR.LG(I).EQ.2) G010 10
2195
            DNAH=RR1*C1(I)
2200
            DNAOH=R3*C2(I)
         11 S1(I)=KK1*QS(I)/M(I)=DNAH
2205
2210
            S2(I)=KK2*QS(I)/M(I)=DNAOH
            S3(I) = KK3 \times QS(I) / M(I) + DNAOH
2215
5550
            S4(I) = KK4 \times QS(I) / M(I) + (DNAH + DNAUH) \times 0.5
2225
         10 CONTINUE
2230 C**** ACCOUNT FOR PUSSIBLE BUBBLE MIGRATION IN THE CCTL VESSEL
2235
            W25=0.
2240
            W26=0.
2245
            WHCT=0.
2250
            WHPU=0.
2255
            IF(C4(25).LE.C4(26)) GOTO 21
            W25=R1 \times (C4(25)-C4(26)) \times M(25)
,5590
         21 IF(C4(26).LE.C4(27)) GOTO 22
2265
2270
            W26=R1*(C4(26)-C4(27))*M(26)
2275
         22 C27=0.5*(C4(27)+C4(26)+0.5*(C1(27)+C1(26)))
2280
            IF(C27.LE.CHNA) GOTO 23
2285
            WHCT=R1*(C27-CHNA)*M(27)
         23 C01=0.5*(C4(1)+C4(30)+0.5*(C1(1)+C1(30)))
2290
2295
            IF(C01.LE.CHNA) GUTO 24
2300
            WHPU=R1 \times (CO1-CHNA) \times M(1)
2305 C**** ACCOUNT FOR CULD TRAP NAH REMODVAL
2310
         24 #42=0.0
2315
            W42(1=0.0)
2320
            IF(LG(42).EQ.0) GOTO 25
2325
            W42=BETA*(C1(42)-C1SAT)
            W420=BETA*(C3(42)-C3SAT)
2330
2335
            IF (w42.LT.0.0) w42=0.0
2340
            IF(W420.LT.0.0) W420=0.0
2345
         25 S4(25)=S4(25)-W25/M(25)
```

```
2350
           S4(26)=S4(26)+(W25-W26)/M(26)
            S4(27) = S4(27) + (W26 - WHUT) / M(27)
2355
           S4(1)=S4(1)-wHPU/M(1)
2360
            S1(42) = S1(42) - W42
2365
            S_3(42) = S_3(42) - W_{420}
2370
           RETURN
2375
            END
2380
2385
                                                                                  -0
2390 [-----
                                                                                  С
2395 C
                                                                                  С
            SUBROUTINE INTEGR.
2400 C
            IN THIS ROUTINE CONCENTRATION OF THE VARIOUS REACTION PRODUCTS
                                                                                   С
2405 C
                                                                                  С
            FOR EACH SEGMENT ARE CALCULATED.
2410 C
                                                                                   C
2415 C
2420 C-----
2425
            SUBRUUTINE INTEGR
2430
            COMMON /BLK/ L,A,M,C1,C2,C3,C4,LG,WS,WCT,WT1,WT2,WT3,WT4,WEX,TEMP,
2435
           C FINTIM, RONA, DIMIN, DIMAX, S1, S2, S3, S4, JT, KS, TPR, IQ, ICT, W, JCT,
2440
           C WR, WA, WX, WB, WC, WD, WE, Q, TQ, TX, QS, PDIS, PH, PA, K1, K2, K3, K4, R1, R2, R3,
2445
           C WHCT, WHPU, TPLEN, VPLEN, IC, TPL, CHNA, RR1, QX, QXT, QHT, C1SAT, BETA,
2450
           C ALFA, TMM, NPICT, NGRAF, NVECT, NAME, IPI, NUDET, NODE, NTYPE,
2455
           C TLAG, CDET, TDLE, C3SAT, PDEL, FIGTTL, PTDL, KH
2460
            COMMON /LOG/ TITLE, PRT1, PRT2, PRT3, PRT4, PRT5
2465
            COMMON /DUB/ TIME, DELT, DC1, DC2, DC3, DC4, ABSC
2470
            REAL*4 L(50),A(50),M(50),C1(50),C2(50),C3(50),C4(50),W(50)
2475
            REAL*4 S1(50),S2(50),S3(50),S4(50),Q(8),TQ(8),TX(8),QS(50)
2480
            REAL*4 K1,K2,K3,K4,KS,TITLE(18),TLAG(7),CDET(7),TDLE(7)
2485
            REAL*8 DC1(50), DC2(50), DC3(50), DC4(50), TIME, DELT, ABSC(4,10)
2490
            LOGICAL PRT1, PRT2, PRT3, PRT4, PRT5
2495
            DIMENSION LG(50), IQ(8), IC(8), ICT(8), NGRAF(10), NVECT(10,5),
2500
           C NAME(10,15), IPI(50), NODE(7), NTYPE(7), FIGTTL(15,10)
2505
2510 C
2515 C**** CALCULATE DERIVATIVES FOR VARIABLES TO BE INTEGRATED AND S*TAU
2520 C**** VALUES FOR PIPE SEGMENTS
2525
            DO 10 I=1,50
            IF(LG(I).EQ.0) GOTO 10
2530
             CC1=0.
2535
2540
             CC2=0.
             CC3=0.
2545
2550
             CC4=0.
2555
            LLG=LG(I)
2560 C**** CALCULATE DERIVATIVES FOR MIXING PLENUM NODES
          5 II=I-1
2565
2570
            IF(I,EQ,1)II=30
            IF(I_EQ_6)II=7
2575
            IF(I_EQ_7)II=5
2580
            GOTO (4,10,4,8,8),LLG
2585
          4 DC1(I)=(W(I)*(C1(II)-C1(I))+CC1)/M(I)+S1(1)
2590
            DC5(I) = (M(I) + (C5(II) - C5(I)) + CC5) + M(I) + S5(I)
2595
            U(3(I) = (W(I) * (C3(II) = C3(I)) + CC3) / M(I) + S3(1)
2600
            DC4(I) = (W(I) * (C4(II) - C4(I)) + CC4) / M(I) + S4(L)
2605
            GUTU 10
2610
```

```
CCTL.FORT
```

2415	C + + + +	MULTIPLE ENTRY NODES
2620	Q X A X A	$\frac{1}{1} \frac{1}{1} \frac{1}$
2020	0	
2023		
2030		
2035		
2040		
2045	-	
2650	1	IF(I.NE.27) GUIU 2
2655		
5660		LC1=W11*L1(50)+W12*C1(48)+W13*L1(48)+W14*L1(46)+WDE1*L1(27)
2665		CC2=W+1*C2(50)+WT2*C2(48)+WT3*C2(48)+WT4*C2(46)+WDET*C2(27)
2670		CC3=WT1*C3(50)+WT2*C3(48)+WT3*C3(48)+WT4*C3(46)=WDET*C3(27)
2675		CC4=WT1*C4(50)+W12*C4(48)+WT3*C4(48)+W14*C4(46)=WDE1*C4(27)
2680		GOTU 4
2685	5	IF(I.NE.29) GUTU 1
5690		CC1=WCT*(C1(43)-C1(28))
2695		CC2=WCT*(C2(43)-C2(28))
2700		CC3=WCT * (C3(43) - C3(28))
2705		CC4=WCT*(C4(43)-C4(28))
2710		GOTO 4
2715	C****	WRONG SEGMENT IDENTIFICATION NUMBER IF PROGRAM ENTERS THIS SECTION
2720	1	PRINT 100,I
2725	10	CONTINUE
2730		DPH=(WHPU+WHCT)*554.0*TPLEN/VPLEN
2735	C****	CALCULATE CONCENTRATION IN SEGMENTS BY INTEGRATION
2740		IP=0
2745		DO 20 I=1,50
2750		LLG=LG(I)
2755		IF(LLG.EQ.0) GUTU 20
2760		IF(LLG.EQ.2) GOTU 21
2765		CALL INTG1(I,C1(I),DC1(I),DELT)
2770		CALL INTG1(I,C2(I),DC2(I),DELT)
2775		CALL INTG1(I,C3(I),DC3(I),DELT)
2780		CALL INTG1(I,C4(I),DC4(1),DELT)
2785		6010 20
2790	21	TAU=M(I)/W(I)
2795		TIM=TIME
2800		DEL=DELT
2805		IF (TAU.GT.TIME) TAU=TIME
2810		IP=IPI(I)
2815		CALL PIPE(TIM, DEL, TAU, IP, FX1, FX2, FX3, FX4)
2820		CALL PIPE(TIM, DEL, TAU, 10, X1, X2, X3, X4)
2825		$S_1(I) = -(X_1 + RR_1)/2 + FX_1$
2830		\$2(I)=-R3*FX2
2835		$s_3(1) = -s_2(1)$
2840		S4(I) = (S1(I) + S2(I)) * 0.5
2845		C1(I)=FX1+S1(I)*TAU
2850		C2(I)=FX2+S2(I)*TAU
2855		C3(I)=FX3+S3(I)*TAU
2860		C4(I)=FX4+S4(I)*TAU
2865		IF(C1(I), LE, 0, 0) C1(I) = 0.0
2870		IF(C2(I), LE, 0, 0) C2(I) = 0.0
2875		IF(C3(I), LE, 0, 0) C3(I) = 0, 0

```
IF(C4(I).LE.0.0) C4(I)=0.0
2880
2885
        20 CONTINUE
2890
           CALL INTG1(1, PH, DPH, DELT)
2895
           RETURN
2900
       100 FURMAT(1H1,///1H ,20('*'), ' ERRUR IN SEGMENT IDENTIFICATION NUMBER
2905
          C, CHECK LG(',I2,') ',20('*'))
2910
           END
2915
-C
2925 C
                                                                               С
2930 C
           SUBROUTINE INTG.
                                                                               С
2935 C
           IN THIS SUBROUTINE THE DERIVATIVES OF THE SYSTEM
                                                                               C
2940 C
           VARIABLES WILL BE INTEGRATED USING EULER INTEGRATION METHOD
                                                                               С
2945 C
                                                                               С
           PARAMETERS:
2950 C
                I - INDEX (FUR FUTURE USE)
                                                                               С
2955 C
                Y - VARIABLE VALUE TO BE INTEGRATED
                                                                               С
2960 C
                DY - DERIVATIVE OF VARIABLE
                                                                               С
2965 C
                DT - DELT - TIME INCREMENT
                                                                               С
2970 C
                                                                               С
2975 C-
2980
2985
           SUBROUTINE INTG1(I, Y, DY, DT)
2990 C
2995
           Y = Y + DY + DT
3000
           RETURN
3005
           END
3010
- C
3020 C
                                                                               С
3025 C
           SUBROUTINE PRIT.
                                                                               С
3030 C
           IN THIS SUBROUTINE THE RESULTS ARE BEING PRINTED
                                                                               С
3035 C
           PERAMETER IPZ =
                                                                               Ç
                            1 PRINT INITIAL CONDITIONS
                                                                               C
3040 C
3045 C
                            2 PRINT A LINE OF SELECTED RESULTS EVERY
                                                                               С
3050 C
                              JTP TIME STEPS
                                                                               C
3055 C
                            3 PRINT FINAL MAP
                                                                               С
3060 C
                                                                               С
3065 C-
                                                                              ---
3070
3075
           SUBROUTINE PRIT(IPZ)
3080 C**** THIS ROUTINE WILL PRINT CONCENTRATION AT ALL SEGMENTS AT TIME T.
3085
           CUMMON /BLK/ L,A,M,C1,C2,C3,C4,LG,WS,WCT,WT1,WT2,WT3,WT4,WEX,TEMP,
3090
          C FINTIM, RUNA, DTMIN, DTMAX, S1, S2, S3, S4, JT, KS, TPR, IQ, ICT, W, JCT,
3095
          C WR, WA, WX, WB, WC, WD, WE, Q, TQ, TX, QS, PDIS, PH, PA, K1, K2, K3, K4, R1, R2, R3,
          C WHCT, WHPU, TPLEN, VPLEN, IC, TPL, CHNA, RR1, QX, QXT, QHT, C1SAT, BETA,
3100
3105
          C ALFA, TMM, NPICT, NGRAF, NVECT, NAME, IPI, NUDET, NDDE, NTYPE,
3110
          C TLAG, CDET, TDLE, C3SAT, PDEL, FIGTTL, PTDL, KH
3115
           COMMON /LOG/ TITLE, PRT1, PRT2, PRT3, PRT4, PRT5
           COMMON /DUB/ TIME, DELT, DC1, DC2, DC3, DC4, ABSC
3120
3125
           REAL*4 L(50),A(50),M(50),C1(50),C2(50),C3(50),C4(50),W(50)
3130
           REAL*4 S1(50),S2(50),S3(50),S4(50),Q(8),TQ(8),TX(8),QS(50)
3135
           REAL*4 K1,K2,K3,K4,KS,TITLE(18),TLAG(7),CDET(7),TDLE(7)
3140
           REAL *8 DC1(50), DC2(50), DC3(50), DC4(50), TIME, DELT, ABSC(4,10)
```



```
3145
           LOGICAL PRT1, PRT2, PRT3, PRT4, PRT5
3150
           DIMENSION LG(50), IQ(8), IC(8), ICT(8), NGRAF(10), NVECT(10,5),
3155
          C NAME(10,15), IPI(50), NODE(7), NTYPE(7), FIGTTL(15,10)
           DIMENSION CHX(10)
3160
3165
           DATA JPR, JTP, JTI/1,0,0/
           TIM=TIME
3170
3175
           GUTU (10,20,30), IPZ
        10 PRINT 300, TITLE
3180
           PRINT 130
3185
           PRINT 140, (I,LG(I),L(I),A(I),M(I),W(I),QS(1),I=1,50)
3190
3195
           PRINT 300, TITLE
           PRINT 100
3200
        22 PRINT 110 ,TIME, JT, FINTIM, DELT, DTMIN, DTMAX, TPR, TPL
3205
3210
           GOTO 21
3215
        30 PRINT 300, TITLE
           PRINT 120
3220
           GOTO 22
3225
        20 IF(ABS(TIM-JPR*TPR)_GT_DELT*0.3) GOTO 90
3230
           JPR=JPR+1
3235
3240
           PRINT 170, TIME, JT
3245
        21 PRINT 180, PH, CHNA, WHPU, WHCT, RR1
3250
           PRINT 190
           PRINT 200, (I, LG(I), DC1(I), DC2(1), DC3(I), DC4(I), S1(I), S2(I), S3(I), S
3255
          C4(I),C1(I), C2(I),C3(I),C4(I),I=1,50)
3260
3265
        25 PRINT 300, TITLE
            IF(IPZ.EQ.3) GOTO 99
3270
3275
           PRINT 230, (ICT(I),I=1,8)
3280
           JTP=0
           JTI=0
3285
3290
        90 JTI=JTI+1
           IF (JTI.LT.JCT) GOTU 99
3295
           JTI=0
3300
           JTP=JTP+1
3305
           DO 91 I=1,8
3310
3315
        91 CHX(I)=(0.5*C1(ICT(I))+C4(ICT(I)))*2.0166/(453.6*1E=6)
           PRINT 220, JT, TIME, PH, QX, QXT, QHT, ALFA, (CDET(I), I=1,4), (CHX(I), I=2,8
3320
3325
          C )
           IF(JTP.GT.50) GOTO 25
3330
3335
        99 RETURN
3340
       100 FORMAT(' *** INITIAL CONDITIONS ***'//)
3345
       110 FORMAT(' TIME
                                                   =',110,' FINTIM =',F10.2,
                               =',F10.2,'
                                            JT
3350
                        =',F10,4,' DTMIN =',F10,5,'
          С
                 DELT
                                                          DTMAX = , F10.4/
              I TPR
                         =',F10.2,'
3355
                                     TPL
                                              =',F10.2)
       120 FORMAT(' *** SIMULATION TERMINATED ***'/)
3360
       130 FORMAT('
                             TYPE',7X, 'SEGMENT PARAMETERS'/
3365
                       SEGM
3370
          C 10X,
                    LENGHT
                                CRUSS-AREA
                                              MASS
                                                          FLOW
                                                                   LEAK (MOL/SEC1/)
3375
       140 FDRMAT(I3,2H *,I3,2X,1P5E11.3)
       190 FORMAT(1H0, ' SEGM TYPE', 7X, 'SEGMENT DERIVATIVES MOL-SEC-LBS', 18X,
3380
3385
          C'SOURCE IN (MOL/SEC)', 19X, 'CONCENTRATION IN (MOL/LIB)'/
3390
              10X.1
                      DC1
                                   DCS
                                             UC3
                                                       DC4
                                                                S1-NAH
                                                                           S2-NADH
          С
3395
                S3-NA20
                             S4-H2
                                     C1-NAH
                                                C2-NAUH C3-NA20
                                                                     C4-H2'/)
          С
       200 FORMAT(I3,2H *, I3, 2X, 1P12E10.3)
3400
       170 FORMAT(1H1, ' SOURCES AND CONCENTRATIONS FUR TIME=',F7.2,' SEC',
3405
```

```
3410
          C ' AT ', 15, '-TH TIME STEP')
3415
       180 FORMAT( ' HYDROGEN PARTIAL PRESSURE IN COVER'
          C ,' GAS PH=',F10.3,' MM-HG',10X,'SIEVERTS EQUILIBRIUM H2 IN NA CHN
3420
3425
          CA=',E12.4,' (MOL/LB)'/' H2 LEAKING FROM THE PUMP TO '
           ,'COVER WHPU= ',E12.4,' MOLS',11X,'H2 TO GAS PLENUM IN',
3430
          С
3435
          C
            1
              CCTL VESEL WHCT=',E11.4,' MOL'/' HYDRID DISSOCIATION RATE RR1='
          C ,11X,E12.4,' SEC-1')
3440
3445
       210 FURMAT (10E12.4)
3450
       220 FORMAT(1X, I5, F6.1, F7.4, 15F7.3)
3455
       230 FURMAT(' STEP TIME PH-(MM) H20-LK TOT LK TOT H2
                                                              ALFA
                                                                    DICTR1 DTC
3460
          CTR2 DTCTR3 DTCTR4 TOTAL HYDROGEN CONCENTRATION IN (PPM) AT NODE #
3465
          C : ',/42X,I2,33X,6(I2,5X),I2)
3470
       300 FORMAT(1H1,20('*'),2X,18A4,2X,20('*'))
           END
3475
3480
----C
3490 C
                                                                             С
           SUBROUTINE SPLOT.
3495 C
                                                                             С
3500 C
           IN THIS ROUTINE DATA WILL BE STURED IN FILE 20 EVERY TPL
                                                                             C
                                                                             ¢
3505 C
           PARAMETER IIP =
                                                                             C
3510 C
                           1 , INITIAL ENTRY
3515 C
                           2 , TIME STEP ENTRY, VALUES STORED
                                                                             C
3520 C
                           3 , FINAL ENTRY, VALUES RETREIVED AND
                                                                             С
3525 C
                                 PRINT-PLOTTED
                                                                             С
3530 C
                                                                             С
3535 C-
                                                                             -0
3540
3545
           SUBROUTINE SPLOT(IIP)
3550 C**** THIS SUBROUTINE WILL STORE DATA OF SPECIFIED CONCENTRATION POINTS
3555 C**** AT PREDETERMAINED SEGMENTS TO BE PLUTTED LATER UN THE TEXTRUNIC
3560 C**** TERMINAL. DATA ARE WRITEN INTO CCTX.DATA≈FT20.F001
3565
           COMMON /BLK/ L,A,M,C1,C2,C3,C4,LG,WS,WCT,WT1,WT2,WT3,WT4,WEX,TEMP,
3570
          C FINTIM, RUNA, DTMIN, DTMAX, S1, S2, S3, S4, JT, KS, TPR, IQ, ICT, W, JCT,
3575
          C WR,WA,WX,WB,WC,WD,WE,Q,TQ,TX,QS,PDIS,PH,PA,K1,K2,K3,K4,R1,R2,R3,
3580
          C WHCT, WHPU, TPLEN, VPLEN, IC, TPL, CHNA, RR1, QX, QXT, QHT, C1SAT, BETA,
3585
          C ALFA, TMM, NPICT, NGRAF, NVECT, NAME, IPI, NUDET, NODE, NTYPE,
3590
          C TLAG, CDET, TDLE, C3SAT, PDEL, FIGTTL, PTDL, KH
           COMMON /LUG/ TITLE, PRT1, PRT2, PRT3, PRT4, PRT5
3595
           COMMON /DUB/ TIME, DELT, DC1, DC2, DC3, DC4, ABSC
3600
3605
           REAL*4 L(50),A(50),M(50),C1(50),C2(50),C3(50),C4(50),W(50)
3610
           REAL*4 S1(50),S2(50),S3(50),S4(50),Q(8),TU(8),TX(8),QS(50)
3615
           REAL*4 K1,K2,K3,K4,KS,TITLE(18),TLAG(7),CDET(7),TDLE(7)
           REAL+8 DC1(50),DC2(50),DC3(50),DC4(50),TIME,DELT,ABSC(4,10)
3620
3625
           LOGICAL PRT1, PRT2, PRT3, PRT4, PRT5
           DIMENSION LG(50), IG(8), IC(8), ICT(8), NGRAF(10), NVECT(10,5),
3630
          C NAME(10,15), IPI(50), NODE(7), NTYPE(7), FIGTTL(15,10)
3635
3640
           DIMENSION CCC(10), VMX(55), VECT(55), LINE(121), IL(5), ILX(5),
3645
             DYD(6), IP(5), YZ(4), YW(4), VEPL(250, 5), VTIM(250)
          С
3650
           LOGICAL L1
3655
           DATA JFL/0/,VMX/55*0./,YZ/0.15,0.2,0.5,1.0/,YW/3.,4.,5.,5./
           3660
3665
           TIM=TIME
3670
           GOTO (10,20,30), IIP
```


3675	10	REWIND 20
3680	20	IF(ABS(TIM-JPL*TPL),GT,DELT*0.3) GOTO 99
3685		JPL=JPL+1
3690	21	DO 5 1=1,8
3695	5	CCC(I) = (0.5 + C1(1)(I) + C4(IC(I))) + 2.0166E + 6/453.6
3700	2	PRD1-MRDHTMRU1
3700		
3/05		EXOL=UNNA/[0.5*U1(2/]+U4(2/)]
5/10		VECTCID=IIM
3715		VECT(2)=ALFA
3720		VECT(3)=QX
3725		VECT(4)=QXT
3730		VECT(5)=WHPT
3735		VECT(6)=EXSC
3740		VECT(7)=PH
3745		VECT(8)=0HT
3750		DO 11 I=1-NUDET
3755	11	VECT(8+T)=CDET(T)
2760	1.1	
2760		1+V 1+V
2777		
5//0		
5/15		VELT(11)=C1(1C(1))
3780		VECT(11+1)=C2(IC(I))
3785		VECT(I1+2)=C3(IC(I))
3790		VECT(I1+3)=C4(IC(I))
3795		VECT(I1+4)=CCC(I)
3800	12	CONTINUE
3805	• -	WRITE (20) VECT
3810		D_{0} 14 I=1.55
2010	• /1	TE (VECT(T) CT VMV(T)) VMV(T)=VECT(T)
2012	14	1F(VECI(1)+GI+VMA(1)) VMA(1)+VECI(1)
3020		
3025	50	PRINT TUU, JPL
3830		DU 26 N=1,NUDET
3835		NN=8+N
3840	26	PRINT 170,NN,N,NTYPE(N),NODE(N)
3845		1=0
3850		DU 25 JPJ=16,51,5
3855		JPM=JPJ+4
3860		I=I+1
3865		PRINT 110, (J1, IC()), J1=JPJ, JPM)
3870	25	CONTINUE
1975	2 3	PRINT 120 (I VMY(I) I=1 EE)
2000	<u>د</u>	FKINI 1207 (1740×(1771=1733)
3000	C	
2002		THIS SECTION PREPARES PRINIPLUT
3890		DU 70 NP=1, NPICT
3895		NG=NGRAF(NP)
3900	C****	FIND MAXIMUM VALUE IN PRESENT PICTURE
3905		YS=0.
3910		DD 60 N=1,NG
3915		ILX(I)=0
3920		N1=NVECT(NP,N)
3025		TE(VMX(N1) CT YS) YS=VMX(N1)
2020	4 م	
2020		CELECT COALE EOD CRARMIC RICINDE
3735	し★★★★	SELEUI SUALE FUR GRAFFIL PIUIURE



3940		D0 61 1=1.11
3945		YM=10, **(I=6)
3950		DO 63 II=1.4
2955		YSC=Y7(11)*YM
3960		DYS=YSC/YW(TT)
3965		$IE(YS_1 I_1YS(1)GOTO_62)$
3970	63	CONTINUE
3975	61	CONTINUE
3980	62	IDY=DYS/YSC+120++0.001
3985	0-	PRINT 130.TITLE
3990		PRINT 180, (FIGITI (I.NP), T=1, 15)
3095		PRINT 140.NP.NG
4000		D0 64 N=1.NG
4005		N1=NVFCT(NP.N)
4010		PRINT 150.N.N1.IP(N).VMX(N1).(NAME(NP. $3*(N=1)+J$).J=1.3)
4015	64	CONTINUE
4020	04	PRINT 220. (ABSC(I.NP), I=1.4)
4025	C+++	PRINT SCALES
4020		ISEO
4030		D(1 65 T±1.121.TD)
		DYD(IS+1)=DYS+IS
4040		IS=IS+1
4050	65	CONTINUE
4055	05	
4060		GUTD (66,67,68), LAB
4065	66	PRINT (166, (DYD(1), 1=1, 1S))
4070	00	
4075	67	PRINT = 167.(DYD(1), I=1.TS)
4080	0,	
4085	68	PRINT 168. (DYD(I), I=1.IS)
4090	69	REWIND 20
4095	C * * * *	SET PROPER SIGNAL CHARACTERS INTO LINE
4100	-	PRINT 210
4105		DO 50 J=1.JPL
4110		READ (20) VECT
4115		VTIM(J)=VECT(1)
4120		DO 52 N=1.NG
4125		N1=NVECT(NP.N)
4130		VEPI(J,N) = VECI(N1)
4135		II (N)=VFCT(N1)/YSC*120
4140		$IF(II(N) F_0) II(N) = 1$
4145	52	CONTINUE
4150		DO 54 I=2,120
4155	54	LINE(I)=IPO
4160	•	DO 56 I=1,121,IDY
4165	56	LINE(I)=ICR
4170		IF (VECT (3).EQ.0.0) GOTO 53
4175		DU 73 I=2,8
4180	73	LINE(I)=IDLR
4185	53	DU 51 N=1,NG
4190		IF(NG.NE.1) GOTO 59
4195		IF(IL(N), EQ, ILX(N)) GUTO 59
4200		IF(IL(N).LT.ILX(N)) GUTU 57

I1=ILX(N)+1

4205

```
4210
           I2=IL(N)
4215
           GUTU 58
4220
        57 I1=IL(N)
4225
           I2=ILX(N)-1
        58 DU 55 I=I1,I2
4230
        55 LINE(I)=IP(N)
4235
4240
        59 LINE(IL(N))=IP(N)
4245
           ILX(N) = IL(N)
4250
        51 CONTINUE
           PRINT 200, VECT(1), LINE
4255
4260
        50 CONTINUE
4265
           PRINT 211
4270
           IF(PRT5) CALL PLUTER(JPL,NP,NG,VEPL,VTIM,YS,TIM,YSC,DYS,FIGTTL,
4275
             ABSC, NAME, NPICT)
          C
4280
        70 CONTINUE
        99 RETURN
4285
4290
       100 FURMAT (1H0,3(/),1H ,20('*'),I6,' RECURDS ARE WRITEN FOR PLUTTING
             ',20('*')//10x, '#01 TIME (SEC).'/10x, '#02 ALFA'/10x,
4295
          C
            1#03 LEAK H20 (MOL/SEC). 1/10X, 1#04
4300
                                                  TUTAL H20 LEAK (MOL) 1/
          С
           10x, #05 H2 FLOW TO PLENUM (MOL/SEC) //10x,
4305
          С
                  EXCESS H2 IN COVER GAS OVER NODE 271/10X,
4310
          С
            #06
4315
          C #07
                  H2 PARTIAL PRESSURE IN CUVER GAS (MM-HG) 1/10X,
4320
          C 1#08
                 TOTAL HYDRUGEN IN COTL SYSTEM (MUL)'/)
       110 FORMAT(' CUNC (MOL/LB) #',12,'
                                            C1(',I2,')=NAH
                                                               #',I2,
4325
4330
             HOAN-(',12,')=NAOH
                                 #',I2,' C3(',12,')=NA20
                                                              #',I2,' C4('
          С
             ,I2,')-H2
                             #',I2,' DETECTABLE H IN NODE ',I2,' (PPM)')
4335
          С
       120 FORMAT('OTHE APPROPRIATE MAXIMUM VALUES OF THE VARIABLES ARE'/
4340
          C 11(11X,5(4X,'#',I2,1PE12.3)/))
4345
       130 FURMAT(1H1,20(!*!),18A4,20(!*!))
4350
4355
       140 FORMAT(' PICTURE #', I2, ' HAS ', I2, ' GRAPHS')
       150 FURMAT(' GRAPH #',12,' IS VECT(',12,'), SYMBOL IS ',A1,' MAX=',
4360
4365
          C E11.4,3X,344)
4370
       166 FURMAT(1X,F10.1,5(14X,1PE10.3))
4375
       167 FURMAT(1X,F10.1,4(20X,1PE10.3))
       168 FURMAT(1X,F10.1,3(30X,1PE10.3))
4380
       170 FORMAT(10x, '#', 12, ' RESPONSE OF DETECTOR ', 12, ' IN (PPM). TYPE'
4385
          C ,'IS ', II, ' CONNECTED TO NODE ', I2)
4390
4395
       180 FORMAT(40X, 15A4)
4400
       200 FORMAT(1X, F7.2, 3X, 121A1)
4405
       210 FURMAT(4x, 'TIME', 3x, 121('_'))
4410
       211 FURMAT(11X,121('-'))
       220 FORMAT(1H0,40X,4A8)
4415
4420
           END
4425
4430
4435 C-----
                                                                             -C
                            4440 C
           SUBRUUTINE PIPE.
                                                                              С
4445 C
           IN THIS RUUTINE PIPE FUNCTION ARE STORED. PIPE LAG FUNCTIONS
                                                                              C
4450 C
           ARE THEN CALCULATED BY LINEAR INTERPOLATION BETWEE THE TWU
                                                                              C
4455 C
           VALUES CLUSEST TO TIME TAU.
                                                                              C
4460 C
           THE PARAMETERS ARE :
                                                                              C
4465 C
                TIME - CURRENT SIMULATION TIME
                                                                              C
```

4470 C DELT - TIME STEP INCREMENT Ç 4475 C TAU - TIME LAG FUR WHICH PIPE FUNCTION IS REQUIRED C 4480 C IP PIPE FUNCTION NUMBER (1-9) C FX1,FX2,FX3,FX4 - CACULATED PIPE FUNCTIONS FOR TIME-TAU С 4485 C 4490 C UR UPDATE VALUES IF TAU=0.0 С 4495 C Ç 4500 C---C 4505 4510 SUBROUTINE PIPE(TIME, DELT, TAU, IP, FX1, FX2, FX3, FX4) 4515 COMMON /LUG/ TITLE, PRT1, PRT2, PRT3, PRT4 4520 LOGICAL PRT1, PRT2, PRT3, PRT4, PRT5 4525 DIMENSION F(10,4,100), CONCN(4), T(100), TITLE(18) 4530 LOGICAL L1,L2 DATA L1,L2/2*.FALSE./,CONCN/'NAH ','NAUH','NA20','H2 11 4535 4540 IF(L1) GOTO 2 4545 L1=.TRUE. 4550 DO 4 I = 1,1004555 T(I) = (I - 100) * DELT * 10.0DO 3 IP=1,9 4560 4565 $F(IP, 1, I) = F \times 1$ 4570 F(IP,2,I)=FX24575 F(IP,3,I)=FX3 4580 $F(IP, 4, 1) = F \times 4$ 4585 **3 CUNTINUE** 4590 **4 CONTINUE** 4595 GOTO 99 4600 2 IF(L2) GOTO 5 4605 L2=.TRUE. 4610 DO 1 I=1,100 4615 $F(10, 1, I) = F \times 1$ 4620 F(10,2,I)=Fx2 4625 F(10,3,I) = FX34630 F(10,4;I) = FX44635 **1 CONTINUE** 4640 GOTO 91 4645 C**** UPDATE THE PIPE FUNCTIONS FOR PRESENT TIME 4650 5 IF(TAU.NE.0.0) GOTO 10 4655 IF(TIME.EQ.T(100)) GOTO 22 4660 DO 8 I=1,99 8 T(I)=T(I+1) 4665 4670 T(100)=TIME4675 22 DU 20 K=1,4 DO 20 I=1,99 4680 4685 20 F(IP,K,1)=F(IP,K,1+1) 4690 F(IP, 1, 100) = FX14695 F(IP,2,100)=FX2 4700 F(IP, 3, 100) = FX34705 F(IP, 4, 100) = FX4GOTO 99 4710 4715 C**** SEARCH FOR PIPE DUTPUT CONCENTRATION AT PRESENT TIME (TIME-TAU) 4720 10 J=04725 DEL=TIME-T(100) 4730 IF(TAU.GT.DEL) GOTO 15

J = 100

4735

```
4740
           TDEL=DEL-TAU
           IF (ABS(TDEL).LT.0.001) GDTU 13
4745
           DTD = (T(100) - T(99) + TDEL) / (T(100) - T(99))
4750
4755
           DP=DTD
4760
           DM=1.-DTD
4765
           GOTO 12
        15 TDEL=TIME-TAU
4770
4775
           IF(TDEL.LT.T(1)) GOTO 90
4780
        9
           J = J + 1
           IF(ABS(T(J)-TDEL).LE.0.001) GUTU 13
4785
4790
           IF(T(J)_GE_TDEL) GOTO 11
4795
           GOTO 9
4800
        11 DT=T(J)-T(J-1)
           DTU=T(J)-TDEL
4805
4810
           DP=DTD/DT
4815
           DM=1.-DP
        12 FX1=F(IP,1,J=1)*DM+F(IP,1,J)*DP
4820
            IF(IP.E0.10) GOTU 99
4825
4830
           FX2=F(1P,2,J=1)*DM+F(1P,2,J)*DP
4835
           FX3=F(IP,3,J=1)*DM+F(IP,3,J)*DP
4840
           FX4=F(IP,4,J-1)*DM+F(IP,4,J)*DP
           GUTO 99
4845
4850
        13 F \times 1 = F(IP, 1, J)
           FX2=F(IP,2,J)
4855
           FX3=F(IP,3,J)
4860
4865
           FX4=F(IP,4,J)
4870
           GOTO 99
4875 C**** ERROR UUTPU[
        91 IF(PRT1) GOTU 92
4880
4885
           GUTU 99
        90 PRINT 100, TIME, TAU, IP, T(1)
4890
        92 PRINT 110,((CUNCN(K),J,T(J),(F(IP,K,J),IP=1,10),J=1,100),K=1,4)
4895
4900
        99 RETURN
       100 FORMAT(1H1,1H ,125('*')/' ERRUR AT TIME=',F10.4/
4905
            ' PIPE DELAY IS TAU=', F10.4, 'PIPE IS SEGMENT NUMBER ', I3/
4910
4915
          C ' FIRST VALUE IN PIPE SEGMENT IS GIVEN AT TIME=',F10.4/1H ,132('*
          C())
4920
       110 FURMAT ('1'/' PIPE FUNCTIONS'/' MAT INDX
4925
                                                          TIME
                                                                   SECT=1',10X,'3
4930
          C',10X,'23',10X,'27',9X,'29',9X,'6',9X,'25',9X,'NU',9X,'NU',6X,'RR1
4935
          C,PH,CHNA'/(1X,A4,I5,0PF12,5,1P10E11.3))
4940
       200 FURMA1 (1x, 3E12, 4, 2I6, 4E12, 4)
4945
           END
4950
4955 C----
                                                                                --C
4960 C
                                                                                 С
4965 C
           SUBROUTINE DETECT.
                                                                                 С
4970 C
            IN THIS ROUTINE THE DIECTOR RESPONSE IS COMPUTED. THREE
                                                                                 С
           TYPES ARE ACCOUNTED FOR: HYDRUGEN IN NA, HYDROGEN IN COVER
                                                                                 Ç
4975 C
                                                                                 С
           GAS, AND DXYGEN. THE RESPONSE IS GIVEN IN PPM WEIGHT FOR THE
4980 C
                                                                                 C
4985 C
           SOLUTION AND PPM-VOLUME FOR THE COVER GAS.
4990 C
                                                                                 C
4995 C----
                                                                                 - C
```

5000		
5005	<u>~</u>	SUBRUUTINE DETECT
5010	L	COMMON AND A N CA CO CO CA CA NO MOT WITH WITH WITH WEN TEMP
5015		$ \begin{array}{c} CUMMUN /DLR/ L, A, M, L, L, L, L, L, L, L, W, W,$
5020	Ĺ	FINITM, KUNA, DIMIN, DIMAX, SI, SZ, SS, S4, JI, KS, IPK, IU, ICI, W, JCI,
5025	C	WR, WA, WX, WB, WC, WD, WE, Q, TQ, TX, Q5, PD15, PH, PA, K1, K2, K3, K4, R1, R2, R3,
5030	C	WHCT, WHPU, TPLEN, VPLEN, IC, TPL, CHNA, RR1, QX, QXT, QHT, CISAT, BETA,
5035	C	ALFA, TMM, NPICT, NGRAF, NVECT, NAME, IPI, NUDEI, NUDE, NIYPE,
5040	C	TLAG, CDET, TDLE, C3SAT, PDEL, FIGITL, PTDL, KH
5045		COMMON /LUG/ TITLE, PRT1, PRT2, PRT3, PRT4, PRT5
5050		CUMMON /DUB/ TIME, DELT, DC1, DC2, DC3, DC4, ABSC
5055		REAL *4 L(50), A(50), M(50), C1(50), C2(50), C3(50), C4(50), W(50)
5060		REAL *4 S1(50),S2(50),S3(50),S4(50),Q(8),TQ(8),TX(8),QS(50)
5065		REAL*4 K1,K2,K3,K4,KS,TITLE(18),TLAG(7),CDET(7),TDLE(7)
5070		REAL*8 UC1(50), DC2(50), DC3(50), UC4(50), TIME, DELT, ABSC(4,10)
5075		LUGICAL PRT1, PRT2, PRT3, PRT4, PRT5
5080		DIMENSION LG(50),IQ(8),IC(8),ICT(8),NGRAF(10),NVECT(10,5),
5085	C	; NAME(10,15), IPI(50), NODE(7), NTYPE(7), FIGTTL(15,10)
5090		TIM=TIME
5095		DEL=DELT
5100		DO 10 N=1,NUDET
5105		LTP=NTYPE(N)
5110		IF(LTP,EQ.3) GUTO 15
5115		N1=NODE(N)
5120		IP=IPI(N1)
5125		TAU=M(N1)/W(N1)+TLAG(N)
5130		IF(TAU.GT.TIME) TAU=TIME
5135		CALL PIPE(TIM, DEL, TAU, IP, FX1, FX2, FX3, FX4)
5140		CALL PIPE(TIM, DEL, TAU, 10, X1, X2, X3, X4)
5145		SD1=-(X1+RR1)/2.*FX1
5150		SD2=-R3*FX2
5155		SD3=-SD2
5160		SD4=-(SD1+SD2)*0.5
5165		CD1=(FX1+SD1*TAU)*1.0083E+6/453.6
5170		CD2=(FX2+SD2+TAU)
5175		CD3 = (FX3 + SD3 + TAU) + 16.0E + 6/453.6
5180		CD4=(FX4+SD4*TAU)*2.0166E+67453.6
5185		GOTO 19
5190	15	CD4=PH*1.0E+6/(PH+PA)
5195	19	GOTU (20,30,40), LTP
5200	C * * * *	HYDROGEN DETECTOR
5205	20	DPP=(CD1+CD4-CDET(N))/TDLE(N)
5210		CALL INTG1(N, CDET(N), DPP, DELT)
5215		GOTO 10
5220	C****	OXIGEN DETECTOR
5225	30	DPP=(CD3-CDET(N))/TDLE(N)
5230		CALL INTG1(N,CDET(N),DPP,DELT)
5235		GOTU 10
5240	C * * * *	HYDRUGEN GAS DETECTUR
5245	40	DPP=(CD4+LDET(N))/TDLE(N)
5250	_	CALL INIGI(N, CDET(N), DPP, DELT)
5255	C****	UTHER TYPES OF DETECTORS
5260	10	CONTINUE

CCTL_FORT

5265 99 RETURN 5270 FND 5275 SUBROUTINE PLOTER(J,NP,NN,X,T,YMX,TF,YSC,DYS,FIGTTL,ABSI,NAME, 5280 C NPICI) 5285 C----• • • C 5290 C С 5295 C SUBRUUTINE PLUTER C 5300 C IN THIS ROTINE A FIGURE UN THE CALCOMP PLOTTER IS PREPARED C C 5305 C PARAMRTERS ARE: 5310 C J - NUMBER OF POINTS IN VECTOR TO BE DRAWN С C C C C 5315 C NP - FIGURE NUMBER 5320 C NN - NUMBER OF CURVES IN FIGURE 5325 C X - VECTOR INCLUDING THE CURVES T - THE TIME VECTOR 5330 C 5335 C YMX - MAXIMUM VALUE OF VECTORS TO BE DRAVN С С TF - TOTAL/FINAL TIME OF THE PLOT 5340 C YSC - SCALE OF THE ABSCISAE C 5345 C C 5350 C HEAD - FIGURE HEADING C 5355 C ABSC - ABSCISAE HEADING С 5360 C NAME - NAME OF CURVES - LEGEND С 5365 C - C 5370 C+ DIMENSIUN x(250,5),T(250),HEAD(15),NAMS(3),TL(2),T1(250) 5375 5380 C ,2(250),NAME(10,15),IPAK(200),FIGTTL(15,10) 5385 REAL*8 ABSI(4,10),ABSC(4) DATA KP/0/ 5390 TF5=TF/5. 5395 5400 TL(1)=TF/25. TL(2)=TF5=TL(1)5405 5410 TI=0. 5415 TX=TF 5420 J1=1 5425 J2=J 5426 C 5427 C**** INSERT ALL TITLES IN PROPER VECTORS FOR PLOTTER DRAWING DO 1 I=1,15 5430 5435 1 HEAD(I)=F1GITL(I,NP) 5440 DO 2 1=1,4 5445 2 ABSC(I) = ABSI(I, NP)5450 IF(NP.GI.1) GUTO 12 CALL STRTPL 5455 5460 12 KP=KP+1 5465 CALL BGNPL(KP) DO 17 N=1,NN 5470 5475 DO 16 K1=1,3 5480 N3=(N-1)*3+K116 NAMS(K1)=NAME(NP,N3) 5485 5490 CALL LINES(NAMS, IPAK, N) 5495 CONTINUE 17 CALL TITLE(1H ,=1,'TIME(SEC)',9,ABSC,32,8.,6.) 5500 5505 CALL HEADIN(HEAD, 100, 3, 1) CALL GRAF (TI, TF5, TX, 0.0, DYS, YSC) 5510 5515 UY=5.3-0.5*NN

5520		(JALL	BL	NK1	(5.	0,7.	8.1	JY,5	5.8,	2)															
5525			CALI	L G	RID	(1,	1)																			
5530			CALI	L F	RAM	Ε																				
5535		1	00 40	0 N	=1,1	NN																				
5540		í	00 10	0 I	=1.	J																				
5545			7(1);	= x {	T N	ì																				
5550	10	í			£	·																				
5555	10		ΣΦΝ 1 Σ + Λ	LIVO	-																					
				ז ר	7 - 1	4 1	`																			
550U			JU 42 T-T-	5 J. 1	2-0	1,0	2																			
2202			12111	1																						
55/0		4	2(1)=	= 2 (;	15)																					
22/2				}≕ •••••	(J) -	J																				
5580		42 1	JUNIJ	INU	Ł																					
5585		1	NW=51	*N+.	20																					
5590			CALI	L C	URVI	E (T	1,2	J	(MV																	
5595	40		CONT	INU	ε																					
5600			CALL	RE	SEI	('B	LNK:	(1)																		
5605		ł	1=270	UY+	0,2																					
5610		(CALL	LE	GEN	D(I	PAK	NN,	5.2	2,01	(2)															
5615			CALL	L E	NDP	L(K	P)																			
5620			IF(KF	P.L	T . N	PIC	1) (OTO	99)																
5625			CALI	L D	ONE	PL																				
5630		99	RETUR	RN																						
5635			END																							
5640	C																									С
5645	Ċ																									č
5650	č		BL	пск	D۵	TΔ																				č
5655	ř		TN	ТН	IS	Rini	TTN		FFAI	н т	AND	01	HE	R 1	TNT	τT	Δ١	ĺλ	T۸	٨	a c	PI	ACE	D		ř
5660	ř			•••					- .		- 10	Ξ,	,,_			. •							~~~			ř
5665	č																									ř
5670	с – ч г																									0
5675	Ŭ		BLO	ск	DAT	۵																				
5680				กิ่ง	ZRI	Ê.	۸ ۱	м. г	^ 1 . r	י כי	7 7	a . i	C I	we	wr	τ.	wτ	ندا _ 1	тэ	. w 1	z	wТ	<u>л</u> . w	EX.T	FMP	_
5685		_ م	ETN	TIM	, PO	NA -	DTM	сы. 1 м. – 1			21 8	2.5	z .	s //	. 1 T		S.	1 7 1	. T	6 .1		Γ. W	. 10	т.	L , , ,	'
5400			- E 1 11 - 14 D - 1	1 ± 13 W A	W Y	u D			J 10) 4 E - 4	4 A F () TV	0.0				.		1 - 14	1 T	נישט שיכי	(Z		100	00	07.	
5405				7 A J 7 W		70 <i>1</i>		1000		4 F F F 7 C	און≰צ ומד	100	1.1.1	013 00	3∦r ⊃1	n /	Г А. О'	ν Τ • Τ	7 R.	с, г т (\] 	, n. 4	141	R.C . T.A	R 31	
57075		- C) / П А Т	MM	NDT					9 1 2 6 2 7 8		T NIN	∦ КГ От	₹ # ₹ 		7 G /		un E	1 # 5 61 T 5		-	,00			
5700		L C			DET	1 10		NGR/	47 J (47 J (אוקן ב דיד	APE		с † 1 С т г			1.00	NUL	E,	14 1 1						
5/05		L		57C	UEI	110	LC/	اد د .			-// + >	001	L /		7 L #	00	16									
5710					10	6/	1111		- R I . - , - , -				31	PR I	14,	PR	10									
5/15			LUMML UFA:	UN .	100		ITW					210	200	,00	4,	AD	るし	• •	~							
5/20			REALS	*4	LO	0),	A (5))),!	9(5)),(1(5	0),	62	(5)	0),	63	(5)	0), ^^	<u><u></u><u></u><u></u><u></u><u></u><u></u><u></u><u></u><u></u><u></u><u></u><u></u><u></u><u></u><u></u><u></u><u></u><u></u><u></u></u>	(5))),	, W (501			
5/25			KEAL	*4	510	201	,82	50.	1,5	5(5))),8	4(5	0)	, 61	(8)	, 1	9(1	5),	IX	(8)	1,6	12(201			
5730		1	REAL	*4	K1,	K2.	K3,1	(4,)	<s,< td=""><td>TIT</td><td>E(1</td><td>8),</td><td>TL</td><td>AG</td><td>(7)</td><td>• C</td><td>DE</td><td>1 (7</td><td>),</td><td>TDL</td><td>Ε(</td><td>(7)</td><td></td><td></td><td></td><td></td></s,<>	TIT	E(1	8),	TL	AG	(7)	• C	DE	1 (7),	TDL	Ε((7)				
5735			REAL	*8	DC1	(50),00	26	50)	,DC:	5(50),U	PC 4	(5)	0),	Ţ1	ME.	, DE	LT	, A E	SSC	:(4	,10))		
5740		I	LOGI	CAL	PR	Τ1,	PRT	2,PF	RT3,	PR'	14,P	RT5			-						_					
5745		1	DIME	NSI	ÛN	LG(50)	,IQ	(8)	,IC	(8),	101	(8),1	NGR	AF	(1)	0),	NV	ECI	[(1	ιο,	5),			
5750		C	NAME	E(1	0,1	5),	IPI	(50)) , N(DDE	(7),	NTY	PE	(7)),F	IG	TT	L (1	5,	10))					
5755	C * *		Df	EFA	ULT	VA	LUE	6																		
5760			DATA	BE	TA/	0.0	01/	,																		
5765		Ç		C 1	SAT	/1.	418	E=6,	/,																	
5770		C		CD	ET/	7 * 0	.01	,																		
5775		C		DT	MAX	/1.	0/,																			
5780		C		DT	MIN	10.	005																			
						-																				



5785	C	JT/0/
5790	DATA	PDEL/0.01/,
5795	С	PRT1, PRT2, PRT3, PRT4, PRT5/5*.FALSE./,
5800	С	Q/8×0.0/,
5805	С	TIME/0,0/,
5810	C	TG/8×10.0/,
5815	С	TX/8*80.0/,
5820	C	WT1,WT2,WT3,WT4/4×0.0/
5825	END	

APPENDIX D

The Input Data; How to Run CCTL-DYSP

1. Title

The first line is a title of 72 characters and will be printed at the top of each output page.

2. INLIST

The data in this section are inserted in a free NAMELIST format. All the data are single variables or vectors, and should be placed between

 $\Delta \& {\rm INLIST} \Delta^{*}$ as a first card, and

 Δ END as the last card.

All the vectors can be input as whole vectors

 $\mathbf{x} = \mathbf{a}_1, \, \mathbf{a}_2, \, \dots, \, \mathbf{a}_{50},$

or single members; e.g.,

 $x(5) = a_5; x(7) = a_7.$

In the first case, all elements of the vectors have to be supplied. (The variables can be input in any order.)

L(50) = CCTL segment length, in feet; LG(50) = a logic variable, which determines the type of segment = 0 the segment is excluded from the simulation = 1 plenum mixing segment = 2 pipe segment = 3 plenum mixing with cover gas = 4 multiple-entry mixing plenum = 5 multiple-entry mixing plenum with cover gas; A(50) = segment cross section area, in ft²; C1(50) = NaH concentration, in ppm; C2(50) = NaOH concentration, in ppm; C3(50) = Na₂O concentration, in ppm. Only the first value for each of C1(1), C2(1), and C3(1), and C4(1) has to be input to calculate the initial distribution in the system.

- Q(8) = leak at the Ith injection point, in lb/sec;
- QT(100) = normalized time-dependent leak function;
 - TQ(8) = time, in seconds, when the leak at node I starts;
- TQT(100) = time table at which normalized leak-function values are given;
 - TX(8) = time (in seconds) when the leak at node I is terminated;
 - IQ(8) = CCTL node number at which leak might occur, i.e., nodes at which nozzles were installed;
 - IC(8) = node numbers for which detailed concentration information will be stored in CCTX.DATA file for future plotting; the nodal information stored includes C1, C2, C3, C4, and detectable hydrogen concentrations, in ppm;
 - ICT(8) = nodes for which hydrogen concentration will be printed every JCT time steps; for ICT(1), however, ALFA will be printed.

3. PARM

The data in this section are system parameters and are inserted in a free NAMELIST format. These are scalar variables. If they will not be included in the input stream, the default value (usually 0) will be assumed by the program. The parameters should be placed between

 Δ PARM Δ as the first card, and

 Δ END as the last card, and should be separated by commas.

- TEMP = sodium temperature, in $^{\circ}F$;
 - WS = total sodium flow, in gal/min;
 - WCT = flow through the cold trap, in gal/min;
 - WT1 = flow toward the detectors from node 6;
 - WT2 = to be determined;
 - WT3 = flow toward the detectors from node 23, in gal/min;
 - WT4 = flow toward the detectors from node 25, in gal/min;

WEX = sodium leak between nodes 3 and 22, in gal/min;

- PDEL = maximum permitted change in node 23 for pipe update;
- PTDL = maximum time interval at which pipe is updated;

- PRT1 = (Logical) if TRUE, initial pipe-function distribution will be
 printed;
- PRT5 = (Logical) if TRUE, time-dependent results arranged for print-plot also will be plotted on the CALCOMP plotter;
- TCLT = Cold-trap temperature;
 - PH = Hydrogen partial pressure in cover gas, in mm Hg;
 - PA = Argon partial pressure in cover gas, in mm Hg;
- FINTIM = simulation time, in seconds;
 - DELT = single integration time step, in seconds;
- DTMIN = minimum permitted time step, in seconds;
- DTMAX = maximum permitted time step, in seconds;
- VPLEN = total gas plenum volume, in ft^3 ;

 - TPL = time intervals at which an entry for plotting is calculated, in seconds;
 - - K1 = fraction of water leak to Na + H₂O \rightarrow NaOH + $\frac{1}{2}$ H₂, reaction;
 - K2 = fraction of water leak to $2Na + H_2O \rightarrow NaOH + NaH$, reaction;
 - K3 = fraction of water leak to $4Na + H_2O \rightarrow 2NaH + Ha_2O$, reaction;
 - K4 = fraction of water leak to $2Na + H_2O \rightarrow Na_2O + H_2$, reaction;
 - R1 = rate of hydrogen disengagement from liquid sodium to cover gas, in sec⁻¹;

BETA = cold-trap static efficiency;

 $R3 = rate of NaOH dissociation, in sec^{-1}$.

4. DTCTR

This section contains a list of parameters describing the detectors monitoring CCTL. Parameters are inserted in free NAMELIST format and should be placed between

 Δ &DTCTR Δ as the first card, and Δ &END as the last card, and should be separated by commas.

- 2 = oxygen detector in sodium
- 3 = hydrogen-gas detector in cover gas;
- TDLE(7) = diffusion time constant for the nickel membrane, in seconds;
- TLAG(7) = time lag between detector sample line inlet and detector, in seconds.

5. Print-Plot Data

These data will direct the printing of time-dependent plots. If TPRS is true, then graphic output on a CALCOMP plotter also will be generated. The data must be input in the formats described below.

	CARD 1	Ξ	The first card can be any comment of up to 80 characters
	CARD 2	=	NPICT;FORMAT(I2), number of pictures to be printed.
	CARD 3	Ξ	NGRAF(10); FORMAT(10(I2, 1X)), NPICT numbers each giving the number of curves to be drawn in a picture.
С	ARD 4-I	=	NVECT(10): FORMAT(10(I2, 1X))

These numbers from 2 to 55 give the position of the variables to be drawn in the 55-place vector VECT as written in the CCTX.DATA file.

#1: time (sec)

- #2: ALFA defined by (C1(I) + C2(I))/average total hydrogen concentration in the loop
- #3: water leak (mol/sec)
- #4: total water leak (mol)
- #5: hydrogen flow to the cover gas (mol/sec)
- #6: excess hydrogen in cover gas over node 27 (mm Hg)
- #7: hydrogen partial pressure in cover-gas plenum (mm Hg)
- #8: total hydrogen in the CCTL system (mol)
- #9-15: detector readings (ppm)
- #16: NaH concentration in the IC(1)th node (mol/lb)
- #17: NaOH concentration in the IC(1)th node (mol/lb)

#18:	Na_2O	concentration	in the	IC(1)th	node	(mol/lb)

- #19: hydrogen concentration in the IC(1)th node (mol/lb)
- #20: detectable hydrogen concentration in the IC(1)th node (ppm)

```
#21-25: same as #16-20, but for IC(2)th node
```

- #26-30: same as #16-20, but for IC(3)th node
- #31-35: same as #16-20, but for IC(4)th node
- #36-40: same as #16-20, but for IC(5)th node
- #41-45: same as #16-20, but for IC(6)th node
- #46-50: same as #16-20, but for IC(7)th node
- #51-55: same as #16-20, but for IC(8)th node
 - CARD 5-I = NAME(10):FORMAT(5(3A4, 1X)): names to be assigned to each curve; must be terminated by \$
 - CARD 6-I = ABSC(10): FORMAT(4A8): 32 alphameric characters to be printed along the abscissa of the picture
 - CARD 7-I = FIGTTL(10):FORMAT(15A4): title to be given to the Ith figure can be up to 60 characters and must be terminated by \$. Card sequences 4-5-6 are repeated NPICT times.
- CARD 8 (A4) = 9999: this is the last card indicating the end of the data input.

A sample input data set is shown below.

6. Sample Input Data Set

```
RUN # 24: CCTLP LEAK DETECTION SIMULATION.(.015LB/SEC AT INJ#4, DUR=5SEC)
 &INLST L=1.,
                40.9.
                         1., 10.,
                                    1.,
                                                   .2775,
                                                             .4171.
                                            1.,
                         .7788,
                                  .8546,
      .4021,
               .4588,
                                            .7788,
                                                     .7221,
                                                               .7221,
               .8546,
                         .7788,
                                  .4588,
                                                               .3889,
      .7788,
                                            .4021,
                                                     .4171,
                                            7,5,
      1.,
               2.89,
                                  2.083,
                                                     19.0,
                         1.0.
                                                               .8,
      31 . ,
      10 + 1.0,
      28.0,
               1.0,
                         16.0,
                                   16 ..
                                             0.0,
                                                      0.0,
                                                                18.585,
               42.67, 42.26,
       36.87,
         1.069,
    A =
                  .09893,
                            .3395,
                                     .09893, .2127,
                                                        1,49,
      16±0.324,
               .09893, 4.03,
                                  6.335.
                                            6.445,
                                                     .15255,
                                                               .15255,
      ,2127,
      .15255,
       10*0.0
      0.00248,
                3.276,
                         0.00248, 1796, .0, .0,
       4*0.00248,
    LG= 3, 2, 1, 2, 1, 16*1,4,1, 2, 2*1, 5, 2, 4, 2, 0, 9*0,
        2, 1, 2, 0, 0, 0, 2, 2, 2, 2,
```

```
C1(1)=75.E-9,
   C2(1)=1.E-9,
   C3(1)=35,E-6,
   C4(1)=1.E=8,
      Q(4) = 0.015,
      Tx(4) = 15.0,
      10(4) = 10.0,
                   17.
                        16,
                             15, 12, 10,
      IQ=22,
             19,
                                            6,
                             47, 1, 27, 29,
              6,
                   49, 23,
      IC=16,
                                  16, 27, 1,
      ICT=47, 6,
                   49,
                        23,
                             47.
KEND
 &PARM TEMP=900., WS=800., WCT=4., WT1=5., BETA=0.9, WT3=5.0, WEX=1.,
 FINTIM=120., DELT=0.05, TPR=20.0, TCLT=240.0, PDEL=0.10,
          PA=800.0, K1=0.45, K2=0.2, K3=0.25, K4=0.1,
                                                            R1=9.625E-6,
  PH=0.1,
    R3=7,5E-5, VPLEN=40., TPL=0.5, JCT=10, PRT5=.TKUE.,
 &END
 &DTCTR NUDET=4,
        NODE(1)=49, NUDE(2)=49, NUDE(3)=47, NODE(4)=27,
        NTYPE(1)=1, NTYPE(2)=2, NTYPE(3)=1, NTYPE(4)=3,
        TLAG(1)=10.0, TLAG(2)=12.0, TLAG(3)=10.0, TLAG(4)=1.0,
        TDLE(1)=14.0, TDLE(2)=15.0, TDLE(3)=14.0, TDLE(4)=10.0,
 &END
***** DATA FUR PRINT PLUT FULLOW. LAST CARD MUST BE 199991 *******
04
04,04,05,02
20,35,40,11
AT NUDE 16 S, AT NUDE 23 S, AT NUDE 47 S, AT NUDE 27 S
HYDROGEN CONCENTRATION IN (PPM)
HYDROREN TRANSIENT CONCENTRATION RESPONSE TO .075LB LEAKS
36,37,38,39
NAH AT # 23$, NAUH AT #23$, NA20 AT #23$, H2 A1 # 23 $
REACTION PRODUCTS CONC. IN (PPM)
CHANGES IN REACTION PRODUCTS IN RESPONSE TU .075 LB LEAK$
09,11,20,45,50
H-DETECTOR1$,H-DETECTOR3$,INJECTOR J4$,PUMP NODE $,CCTL VESSEL$
HYDROGEN CONCENTRATION IN (PPM)
DETECTOR READINGS RESULTING FROM .075LB LEAK-INJECTOR J45
10,12
H-DETECTOR2$,0-DETECTUR4$
DETC2 IN (WPPM); DETC4 IN (VPPM)
H-DETECTORS READING IN COVER GAS AND STEAM GENERATUR TUPS
9999
/*
```

ACKNOWLEDGMENTS

I extend my thanks to L. F. Epstein, R. A. Jaross, and J. M. McKee for their constructive comments and discussions during this study.

REFERENCES

- 1. R. A. Jaross, Work Plan for Steam Generator Leak Detector Tests in CCTL, T0022-0002-SA-00 (Mar 29, 1973).
- 2. E. S. Amis, Kinetics of Chemical Change in Solution, McMillan Co., N. Y. (1949).
- 3. P. B. Longton, Reactions of Alkali Metals with Gases; Part VI: The Reaction of Sodium with Hydrogen, IGR-TN/C.435 (1957).
- 4. A. K. Fischer, "Studies of Oxygen-Hydrogen Interaction in Sodium: Isotope-exchange Studies," Sodium Technology Quarterly Report: January-March 1972, ANL-7944, pp. 41-44 (Aug 1972).
- 5. D. N. Rodgers and D. Dutina, Recommended Values for NaH Dissociation and the Solubilities of Oxygen and Hydrogen in Sodium, NEDM-12473 (July 1974).
- 6. G. Naud, Contribution to the Study of Hydrogenated and Oxygenated Impurities in Liquid Sodium, CEA-R-2583 (1964).
- 7. P. B. Longton, Reactions of Alkali Metals with Gases; Part VII: Reaction of Sodium with Water Vapor, IGR-TN/C.418 (1956).
- 8. D. D. Adams, G. J. Barenborg, and W. W. Kendall, Evaluation of the Sodium-Water Reaction in Heat Transfer Systems, KAPL-P-1512 (1956).
- 9. D. R. Vissers, J. T. Holmes, and P. A. Nelson, A Hydrogen Activity Meter for LMFBRs, Trans. Am. Nucl. Soc. 14(2), 610-611 (1971).
- P. Vilinskas, "Calculated Hydrogen-Oxygen Equilibria in Liquid Sodium," Proc. Int. Conf. Sodium Technology and Large Fast Reactor Design: November 7-9, 1968, ANL-7520, Part 1, pp. 477-480.
- 11. M. D. Banus, J. J. McSharry, and E. A. Sullivan, Sodium-Sodium Hydride-Hydrogen System at 500-600°C, J. Am. Chem. Soc. 77, 2007-2010 (1955).
- 12. H. C. Pellow, A Model to Predict the Effect of Hydrogen Sources on an LMFBR Steam Generator Leak Detection System, NEDM-13992 (July 13, 1973).
- 13. J. Birault et al., Detection of Small Leaks by Hydrogen Measurements in a Sodium-Heated Steam Generator, Proc. Int. Conf. Sodium Technology and Large Fast Reactor Design, ANL-7520 (1968), Part 1, pp. 345-373.