860924

ORNL CONTAINMENT IODINE MODEL

E. C. BEAHM

C. F. WEBER

T. S. KRESS

R. J. ANDERMANN

1

TRENDS

(TRANSPORT AND RETENTION OF NUCLIDES IN DOMINANT SEQUENCES)

- WHAT IT DOES
- HOW IT WORKS
- MODELS AND DATA
- CALCULATIONS OF SPECIFIC SEQUENCES

ORNL WS 42178

ORNL IODINE MODEL

- DISTRIBUTES IODINE AS I_2, HI, CH_3I, CsI, I^-, AND AgI
- ALLOWS PHYSICAL TRANSFER BETWEEN PHASES OR LOCATIONS
- ALLOWS CHEMICAL TRANSFER BETWEEN IODINE CHEMICAL FORMS

SPECIE	PHASES CONSIDERED
I_2	GAS, AEROSOL, LIQUID, SURFACES (PAINT, STEEL, CONCRETE) DEPOSITED AEROSOL
CH_3I	GAS, LIQUID, SURFACE (PAINT)
CsI OR I^-	GAS, AEROSOL, LIQUID, SURFACES, DEPOSITED AEROSOL
HI	GAS, AEROSOL, SURFACE (STEEL), DEPOSITED AEROSOL
AgI	PRECIPITATE

20 INVENTORY LOCATIONS ARE FOLLOWED WITHIN EACH CONTAINMENT VOLUME.

ORNL IODINE MODEL

TRANSFER BETWEEN PHASES AND CHEMICAL REACTIONS ARE EXPRESSED IN THE GENERAL FORM:

$$\frac{dN_{ix}}{dt} = \alpha^{i}_{xy} N_{ix} - \beta^{i}_{xy} N_{iy}$$

WHERE

N = GRAM-ATOMS OF IODINE,

i = THE IODINE CHEMICAL FORM, I.E., I_2, CH_3I, ETC.,

x,y = THE PHASE LOCATION, I.E., GAS, AQUEOUS, OR SURFACES,

α,β = RATE COEFFICIENTS FOR THE ADDITION OR REMOVAL OF THE SPECIES.

ORNL WS 42167

DEPOSITION/REVAPORIZATION
STEEL, PAINT, CONCRETE, AEROSOL

RATE EQUATION:

$$\frac{dC_s}{dt} = vC_g - \tilde{v}\ C_s,$$

WHERE

C_g = GASEOUS IODINE CONCENTRATION, g-mol/cm^3;

C_s = SURFACE IODINE CONCENTRATION, g-mol/cm^2;

v = DEPOSITION VELOCITY, cm/s;

$\tilde{v}$ = REVAPORIZATION RATE CONSTANT, s^{-1}

REMOVAL OF VAPOR SPECIES BY CONDENSING STEAM (DIFFUSIOPHORESIS)

$$\partial C_I = - \left[\frac{X_S}{X_S + X_A \sqrt{M_A/M_S}} \right] \frac{Q_S C_I}{V}$$

WHERE

C_I = CONCENTRATION OF SPECIES I,

X_S = MOLE FRACTION OF STEAM IN THE CONTAINMENT ATMOSPHERE,

X_A = MOLE FRACTION OF NONCONDENSABLES IN THE CONTAINMENT ATMOSPHERE,

M_S = MOLECULAR WEIGHT OF STEAM,

M_A = AVERAGE MOLECULAR WEIGHT OF THE NONCONDENSABLES,

V = CONTAINMENT CELL VOLUME,

Q_S = VOLUMETRIC STEAM CONDENSATION RATE ONTO THE PARTICULAR SURFACES.

MASS TRANSPORT TO/FROM PARTICLE SURFACES

$$Sh_I \equiv \frac{h_p D}{\mathcal{D}_I} = 2 \text{ (LIMIT FOR DIFFUSIONAL TRANSPORT)}$$

WHERE

Sh_I = SHERWOOD NUMBER,

D = AEROSOL PARTICLE DIAMETER,

$\mathcal{D}_I$ = DIFFUSION COEFFICIENT FOR SPECIES I,

h_p = MASS TRANSPORT COEFFICIENT.

TRANSPORT TO CONTAINMENT SURFACES

FOR LAMINAR FLOW CONDITIONS:

$$Sh = 0.54\,(ScGr)^{1/4}$$

AND FOR TURBULENT CONDITIONS

$$Sh = 0.14\,(ScGr)^{1/3}$$

WHERE

Sh_I (SHERWOOD NUMBER) $\equiv \dfrac{H_I\,L}{\mathcal{D}_I}$

L = A CHARACTERISTIC LENGTH OF THE SURFACE,

$\mathcal{D}_I$ = DIFFUSION COEFFICIENT FOR SPECIES I,

Sc_I = (SCHMIDT NUMBER) $\equiv \mu/\rho\,\mathcal{D}_I$,

μ = VISCOSITY OF CONTAINMENT ATMOSPHERE,

ρ = DENSITY OF CONTAINMENT ATMOSPHERE,

Gr = (GRASHOF NUMBER) $\equiv \dfrac{g\Delta T L^3 \rho^2}{T_G\,\mu^2}$

g = GRAVITATIONAL ACCELERATION,

$\Delta T = [T_G - T_W]$,

T_G = BULK ATMOSPHERE GAS TEMPERATURE,

T_W = WALL SURFACE TEMPERATURE.

CONVECTION BETWEEN VOLUMES OR LEAKAGE

$$\frac{\partial C_I}{\partial T} = -\sum_J \frac{Q_J C_I}{V}$$

WHERE Q_J IS THE VOLUMETRIC FLOW OUT PATHWAY J AND V IS THE VOLUME OF THE CELL (CONTAINMENT OR SUBCOMPARTMENT), AND C_I IS GAS CONCENTRATION.

ENFORCED EQUILIBRIA

I_2 (AQUEOUS) $\rightleftarrows$ I_2 (GAS)

CH_3I (AQUEOUS) $\rightleftarrows$ CH_3I (GAS)

I_2 ADSORPTION ONTO AEROSOLS – LANGMUIR

ISOTHERM

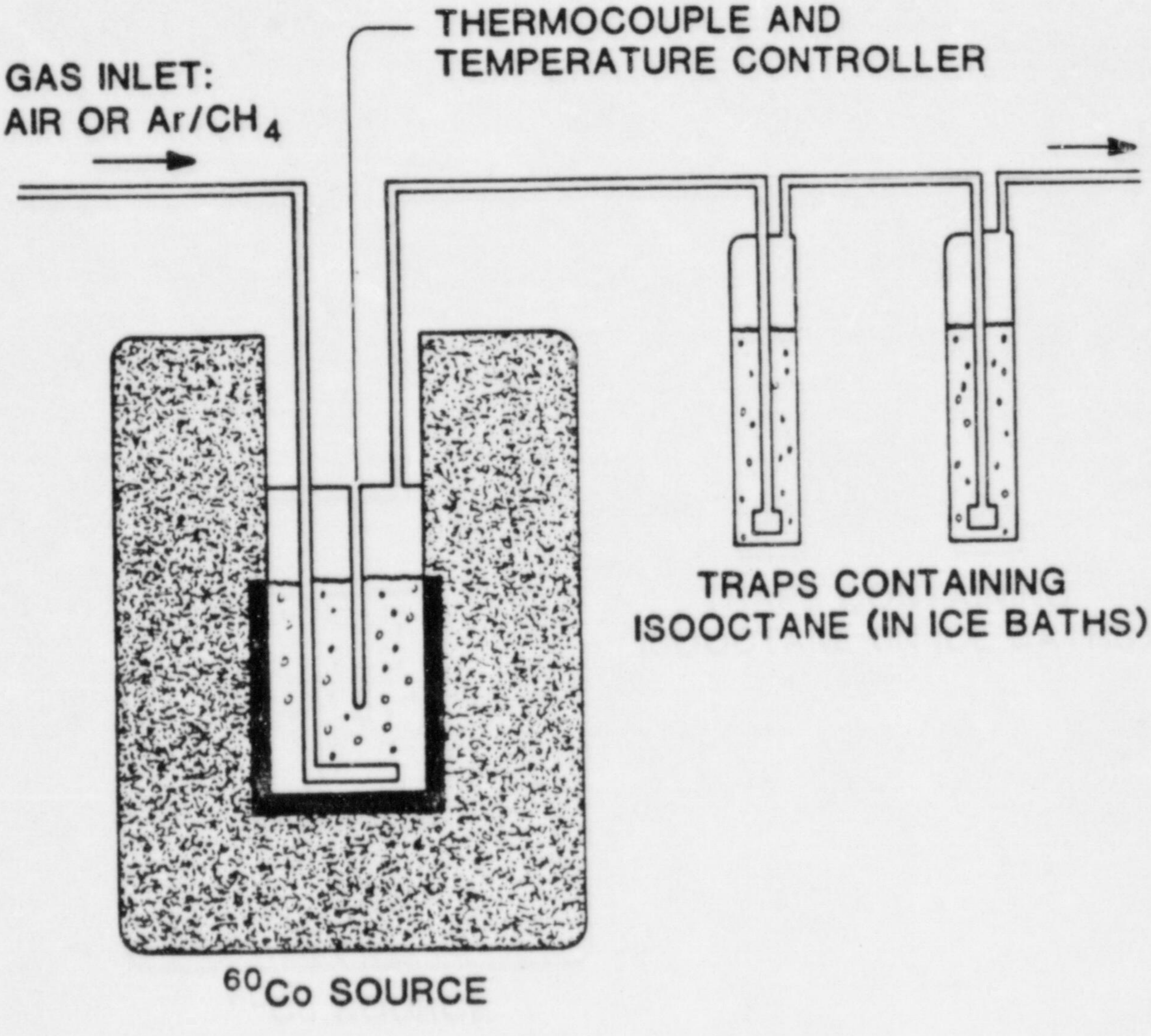
VOLATILITY

- EVALUATION OF pH
- VOLATILITY MEASUREMENTS FOR SPECIFIC ACCIDENT SEQUENCES
- CALCULATION OF RADIATION DOSE RATES
- MODELING OF I^- TO I_2 CONVERSION (RADIATION EFFECT)

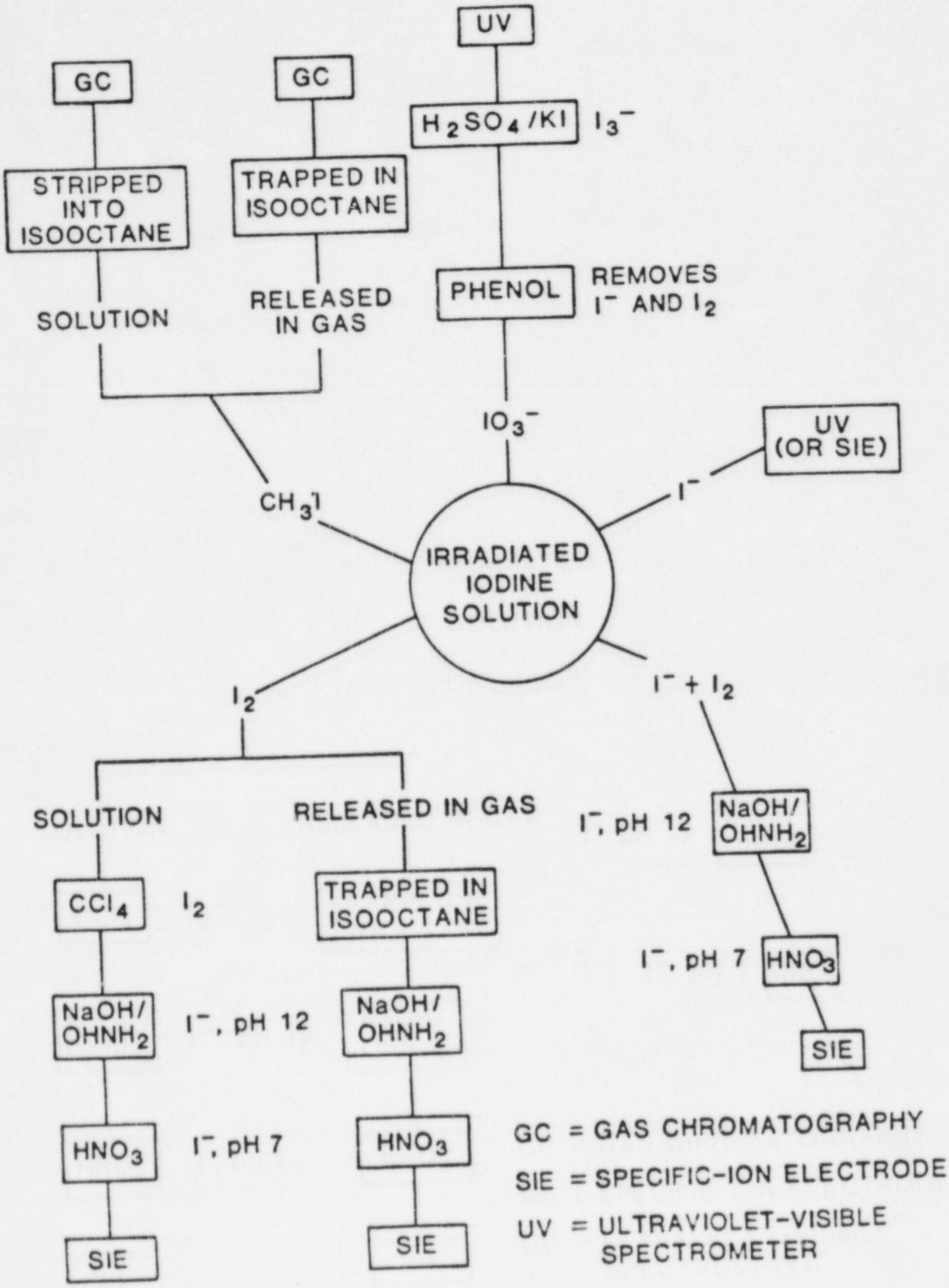
DETERMINATION OF pH

- BORON OXIDES
- BASIC FISSION PRODUCT COMPOUNDS SUCH AS CESIUM HYDROXIDE OR CESIUM BORATES
- IODINE AS HI
- pH ADDITIVES
- ATMOSPHERIC SPECIES SUCH AS CARBON DIOXIDE, NITRIC ACID, OR AMMONIA
- ALKALI AND ALKALINE EARTH OXIDES FROM CORE-CONCRETE AEROSOL

ORNL DWG 86-564



EXPERIMENTAL APPARATUS



ANALYTICAL SCHEME

HI SENSITIVITY STUDY

- SURRY TMLB'ϵ — LATE CONTAINMENT FAILURE
- SURRY TMLB'δ — EARLY CONTAINMENT FAILURE
- PEACH BOTTOM TC

CONVERSION TO I_2

pH	6.8	6.1	3.05
$[I^-]/M$	1.1×10^{-4}	8.6×10^{-4}	8×10^{-4}
RADIATION DOSE/MR	% CONVERSION TO I_2		
0			0.15
0.28			26.1
0.63		0.14	48.1
0.70	0.39		
2.0	0.30	0.33	72.0
3.5	0.22		
4.0		0.50	

EXPERIMENTAL CONDITIONS: 0.05 M BORIC ACID

92°C

0.62 MR/H

AIR PASSED OVER SOLUTION

RADIATION DOSE EFFECT:

pH 4.4, 3×10^{-5} G-AT. I^-/L, 3.9×10^{-4}, MOLS CH_4/L AT 92°C

RADIATION DOSE MRAD	% CONVERSION TO CH_3I
0.31	1.3
0.62	2.0
1.90	3.7
3.10	8.4

CONVERSION OF IODIDE ION TO METHYL IODIDE FROM IRRADIATION OF SOLUTIONS CONTAINING ORGANIC MATERIALS: INITIAL I^- CONCENTRATION, 5.4–7.6 × 10^{-4} <u>M</u>, pH 3.0–3.1, AT 92°C

ORGANIC MATERIAL	RADIATION DOSE IN MEGARAD	PERCENT OF INITIAL I^- CONVERTED TO CH_3I
ETHYLENE PROPYLENE RUBBER, 10.4 G IN 100 ML	0.5	0.15
ETHYLENE PROPYLENE RUBBER, 10.4 G IN 100 ML	1.0	0.27
ETHYLENE PROPYLENE RUBBER, 2.1 G (CUT INTO SMALL PIECES) IN 100 ML	1.0	0.45
ETHYLENE PROPYLENE RUBBER, 11 G IN 100 ML	2.0	1.0
STAINLESS STEEL TURNINGS, IN 100 ML	2.0	0.15
DOWEX 50 CATION EXCHANGE RESIN, 0.1 G IN 100 ML	2.0	0.34

GAS-SURFACE CONVERSION TO CH_3I:

2.4×10^{-4} MOL CH_4/L GAS, 92°C

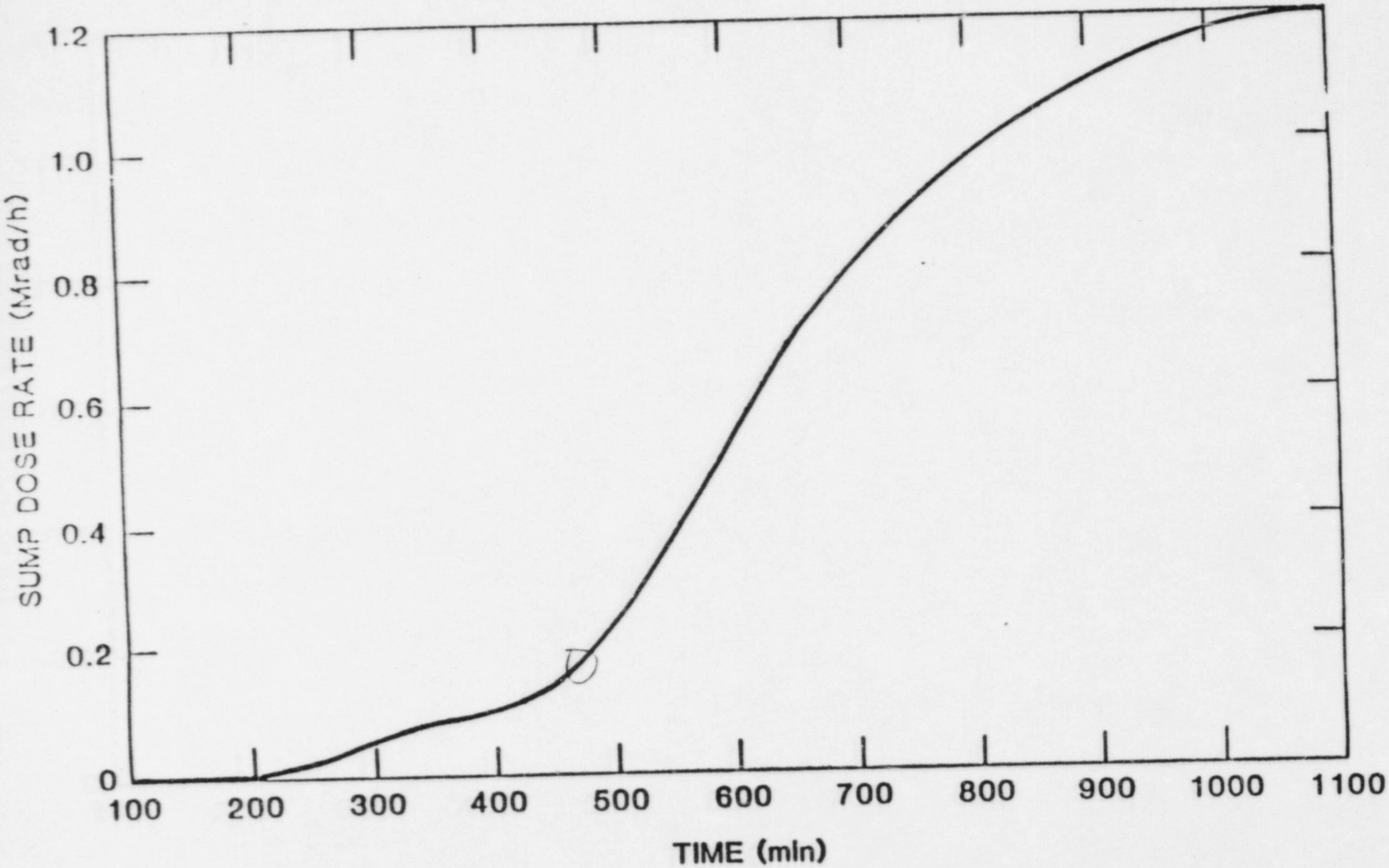
pH	6.1	3.05
$[I^-]$ (MOL/L)	1×10^{-4}	8×10^{-4}
RADIATION DOSE (10^6 RADS)	PERCENT CONVERSION TO CH_3I	
0.5	0.1	0.2
1.0	0.1	0.5
2.0		0.6

RADIATION LEVEL FOR WATER POOLS

SUMP DOSE FOR SURRY TMLB' SEQUENCE

	GROUP	RELATIVE DOSE (MRAD/G-H)
TE	1	1.112E-05
I	2	2.309E-04
CS	3	3.187E-06
RU	4	6.533E-06
CE	5	1.414E-06
LA	6	1.987E-05
SR	7	2.475E-05
ZR	8	1.208E-05
NB	9	6.035E-04
MO	10	3.651E-06
BA	11	8.457E-06
SB	12	2.699E-03
KR	13	7.846E-06
XE	14	1.745E-06

ORNL DWG 86-565



SUMP DOSE RATE FOR SURRY TMLB' SEQUENCES

THERMAL HYDRAULIC AND TRANSPORT DATA

(1) BMI-2104, volume 5
(2) NAUA-4 computer code runs supplied by Battelle Columbus Laboratory
(3) TRAPMELT2 computer code runs supplied by Battelle Columbus Laboratory
(4) ORNL SASA program calculations

The following input data, parameters, and computer code generated results are used:

(1) Control volume parameters
- (a) containment volume
- (b) containment surface area for aerosol sedimentary deposition
- (c) containment surface area for aerosol diffusional deposition

(2) Aerosol source function versus time
- (a) release rate
- (b) cesium iodide fraction

(3) Containment temperature versus time

(4) Containment pressure versus time

(5) Sumpwater temperature versus time

(6) Leakrate out of containment versus time

(7) Steam condensed to the wall versus time

(8) Aerosol data versus time
- (a) Airborne mass
- (b) Accumulated sedimentary deposit
- (c) Accumulated diffusional deposit
- (d) Items a, b, and c for condensed water
- (e) Items a, b, and c for "dry" particles
- (f) Items a, b, and c for cesium iodide
- (g) Particle concentrations
- (h) Average particle radius
- (i) Average particle density
- (j) Particle radius frequency distribution

(9) Cesium iodide total core release versus time

(10) Cesium iodide reactor coolant system retention

MODEL FOR I^- TO I_2 CONVERSION WITH RADIOLYSIS

FOR A GIVEN pH:

$$X(D) = A(1 - e^{-BD})$$

WHERE

X(D) = MASS FRACTION OF I_2 FORMED.

D = RADIATION DOSE,

A,B = CONSTANTS.

PRINCIPAL IODINE REPOSITORIES AT END OF SURRY TMLB'E SEQUENCE

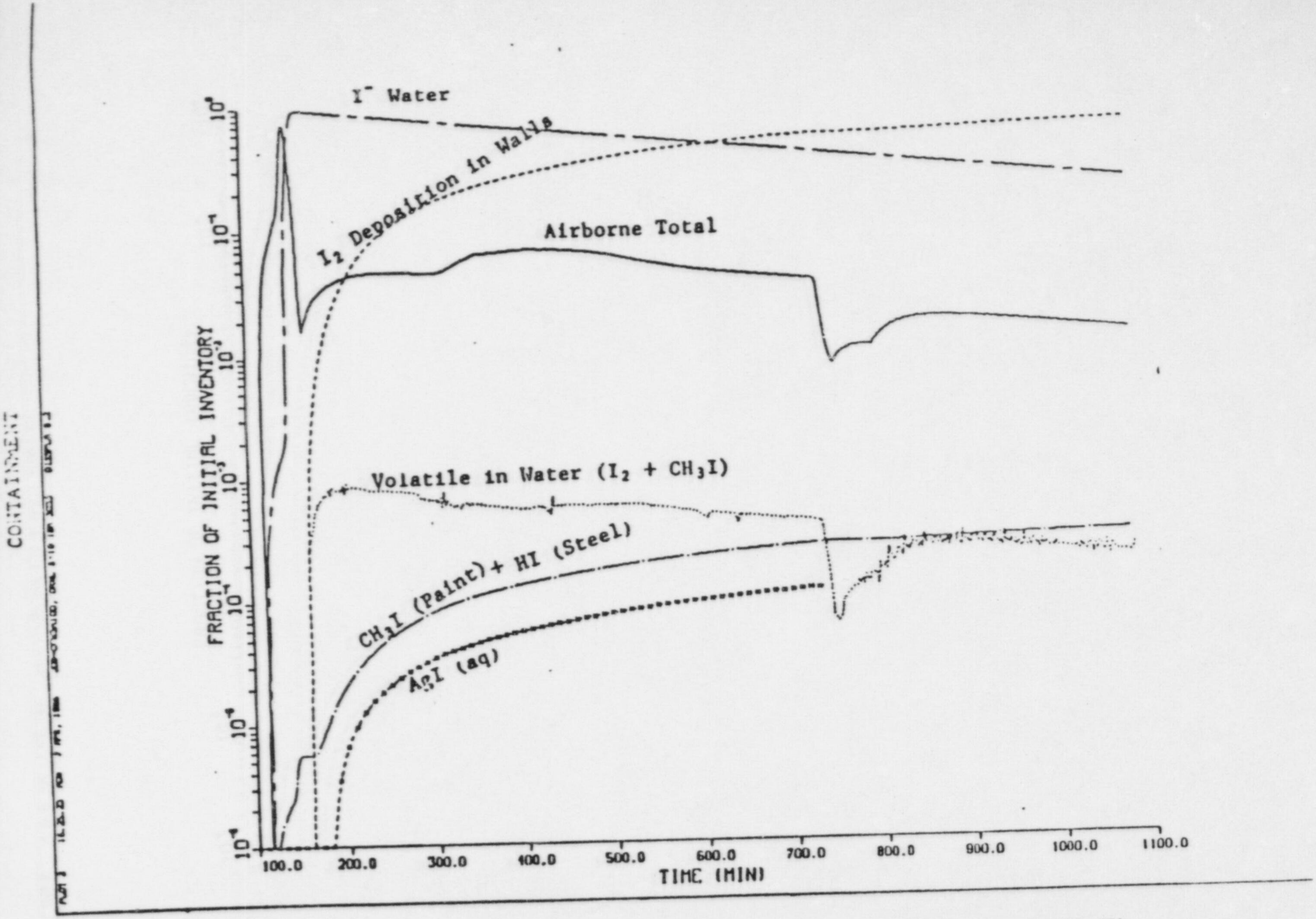
(PWR-Station Blackout with late containment failure)

Location	Iodine Inventory (percent of core inventory)			
	BMI-2104	I[a]	II[b]	III[c]
Airborne in Containment		.02	.09	1.41
Dissolved in Containment Sump		16.43	99.40	23.04
Deposited on Containment Surfaces		10^{-4}	.02	69.46
Released to Atmosphere				
Aerosol	.28	.31	.47	2.12
Gaseous		10^{-6}	10^{-4}	4.07

[a] Same conditions as BMI-2104: pH=6.8, No HI, total iodine release into containment of 2.1 kg.

[b] All iodine retained by the RCS in BMI-2104 is released as HI; total iodine release to containment of 12.7 kg; pH=6.1.

[c] All iodine released as HI, total iodine release to containment of 12.7 kg; pH=3.05.



Distribution of iodine in containment, Surry TMLB'ε, low pH (3.05).

Surry TMLB'δ (Station Blackout with early containment failure)
Principal iodine repositories at end of sequence

	Iodine inventory (percent of initial core inventory)			
	BMI-2104	I[a]	II[b]	III[c]
Airborne in containment		0.01	0.03	0.53
Dissolved in containment sump		15.5	72.9	17.0
Deposited on containment surfaces		0.01	0.1	51.2
Released to atmosphere				
Aerosol	7.0	8.32	26.74	27.38
Gaseous		10^{-4}	0.27	3.87

[a]Same conditions as BMI-2104: pH = 6.8, no HI, total iodine release into containment of 2.1 kg.

[b]All iodine retained by the RCS in BMI-2104 is released as HI; total iodine release to containment of 12.7 kg; pH = 6.1

[c]All iodine released as HI, total iodine release to containment of 12.7 kg; pH = 3.05.

RESULTS OF SURRY TMLB'δ SEQUENCE CORRECTED TO ELIMINATE WASHOUT

Principal iodine repositories for the Surry TMLB'δ sequence[a]

Location	Iodine inventory (percent of core inventory)			
	BMI-2104	I[b]	II[c]	III[d]
Airborne in containment		0.1	0.2	0.6
Dissolved in containment sump		2.4	46.6	12.4
Deposited on containment surfaces		10^{-5}	0.05	35.96
Released to atmosphere				
Aerosol		21.3	53.9	48.1
Gaseous		10^{-6}	0.02	3.0

[a] Corrected to eliminate massive condensation on and washout of aerosols.

[b] Same conditions as BMI-2104: pH = 6.8, no HI, total iodine release into containment of 2.1 kg.

[c] All iodine retained by the RCS in BMI-2104 is released as HI; total iodine release to containment of 12.7 kg; pH = 6.1

[d] All iodine released as HI, total iodine release to containment of 12.7 kg; pH = 3.05

RESULTS OF PEACH BOTTOM TC2 CALCULATIONS

Principal iodine repositories

Location	Principal iodine repositories (% of core inventory)				
	I	II	III	IV	BMI
Drywell					
Airborne	0.03	0.03	0.005	0.005	
Surfaces	4.5	4.5	0.3	0.3	
Wetwell					
Airborne	0.2	0.2	0.03	0.03	
Surfaces	18.4	18.4	1.4	1.4	
Water	51.3	51.3	87.5	87.5	
Reactor building					
Airborne	0.04	0.05	0.008	0.011	
Surfaces	10.1	13.3	2.1	2.9	
(Note: no water pools)					
SGTS[a]					
Charcoal	1.4	0	0.02	0	
HEPA	3.5	0	1.4	0	
Atmosphere					
Gas	1.8	2.2	0.02	0.03	
Aerosol	2.9	3.9	1.2	1.8	1.3

Cases: I = low pH (4.4), SGTS operating
II = low pH (4.4), no SGTS
III = high pH (7.8), SGTS operating
IV = high pH (7.8), no SGTS

[a]Standby Gas Treatment System.