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The Absorption of Gaseous Iodine by Water Droplets

M. F. Albert

Prepared for the U.S. Nuclear Regulatory Commission
Office of Nuclear Regulatory Research
Under Interagency Agreements DOE 40-551-75 and 40-552-75

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THE ABSORPTION OF GASEOUS IODINE BY WATER DROPLETS

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ABSTRACT

A new model has been developed for predicting the rate at which gaseous molecular iodine is absorbed by water sprays. The model is a quasi-steady state mass transfer model that includes the iodine hydrolysis reactions. The parameters of the model are spray drop size, initial concentration of the gas and liquid phases, temperature, pressure, buffered or unbuffered spray solution, spray flow rate, containment diameter and drop fall height. The results of the model were studied under many values of these parameters. Plots of concentration of iodine species in the drop versus time have been produced by varying the initial gas phase concentration of molecular iodine over the range of 1×10^{-5} moles/liter to 1×10^{-10} moles/liter and a drop size of 1000 microns.

Results from the model are compared to results available from the Containment Systems Experiments at Pacific Northwest Laboratory. The difference between the model predictions and the experimental data ranges from -120.5% to 68.0% with the closest agreement 7.7%. The new spray model is also compared to previously existing spray models. At high concentrations of gaseous molecular iodine, the new spray model is considered to be less accurate but at low concentrations, the new model predicts results that are closer to the experimental data than the model called the realistic model from WASH-1329. Inclusion of the iodine hydrolysis reactions is shown to be a feature important to a model intended for determining the removal of molecular iodine over a wide range of conditions.

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1. BACKGROUND

1.1 Introduction

To minimize the release of radioactive iodine to the environment under the conditions of the design basis accident, all light water reactors have a containment water spray system. The spray systems are located outside of the reactor vessel and inside the primary containment for both PWR and BWR designs. Figure 1 shows the location of the containment sprays for the BWR Mark I containment design.[1] The purposes of the spray systems are to remove the heat and thereby lower the pressure within the primary containment and to remove airborne fission products. PWR spray systems employ a buffered water solution while BWR spray systems employ ordinary water taken from the pressure suppression pool.

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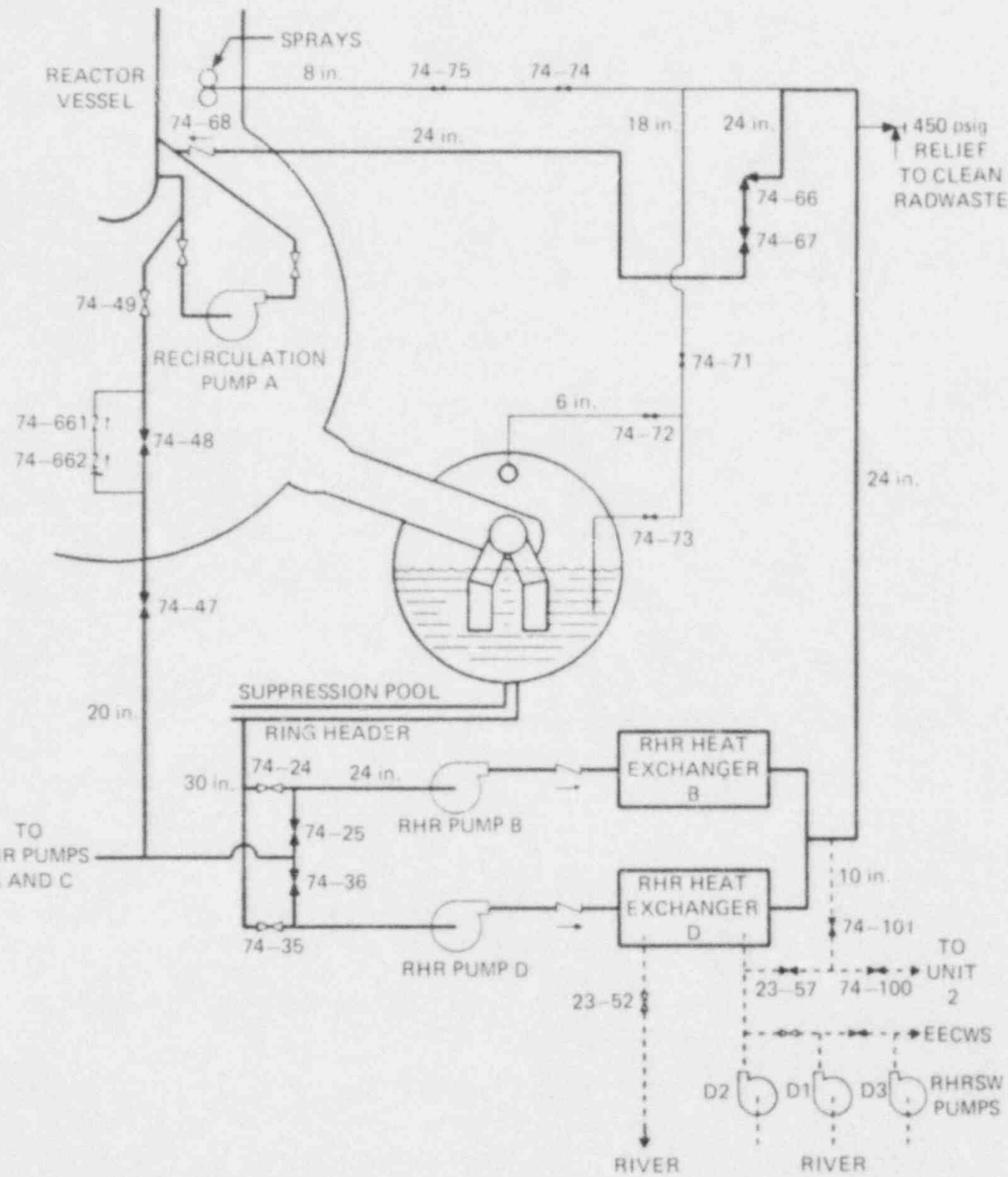

Fig. 1. One Loop of the Residual Heat Removal (RHR) System for the BWR MARK I Containment. Containment Spray is one of the seven operating modes of this system.

Models that predict the rate of iodine removal by the containment sprays are necessary for rational design of spray systems and for predicting the behavior of existing spray systems under accident conditions.

The objectives of this work are to develop a new model for the absorption of gaseous molecular iodine by water droplets which includes the iodine hydrolysis reactions and to determine if and under what conditions, the iodine hydrolysis reactions influence the rate of mass transfer. The parameters of the model are the initial gas phase concentration of molecular iodine, the initial concentration of the iodine

species in the liquid (including pH), the gas phase temperature, the liquid phase temperature, the pressure, the diameter of the droplets, the spray flow rate, the spray time, the containment diameter and the containment height (drop fall height).

1.2 Existing Spray Models

The spray solutions used for PWR spray systems are, for the most part, sodium hydroxide-boric acid solutions, while ordinary water is used in BWR spray systems. The existing model[2] for the removal rate of iodine is first order and can be expressed by:

$$\frac{dC}{dt} = -\lambda C \, , \tag{1}$$

where

C = concentration of iodine in the gas phase,
t = time,
λ = washout rate constant.

Integrating:

$$C = C_o \exp(-\lambda t) \tag{2}$$

where C_o is the initial iodine concentration.
The washout rate constant is defined as:

$$\lambda = \frac{F\ P\ E}{V} \, , \tag{3}$$

where

F = spray flow rate,
$P = \frac{C_l}{C_g}$ = iodine partition coefficient for iodine between water and air (related to Henry's coefficient),
V = containment volume, and
E = removal efficiency.

The removal efficiency is defined as:

$$E = 1 - \Sigma \; \frac{6 N_{Sh}{}^2 \exp(-a_n^2 \, \Phi)}{a_n^2 (a_n^2 + N_{Sh}(N_{Sh} - 1))} \text{ for a stagnant drop model ,} \tag{4}$$

$$E = 1 - \exp\left[-\frac{6k_g t_e}{d(P + k_g/k_l^o)}\right] \text{ for a stagnant film model }, \tag{5}$$

$$E = 1 - \exp\left[-\frac{6\ k_g\ t_e}{d\ P}\right] \text{ for a well-mixed model }, \tag{6}$$

and

$$E = \frac{6\ k_g\ h}{P\ v_g d} \text{ for a gas phase controlling resistance model }. \tag{7}$$

In these equations,

k_g = gas film mass transfer coefficient,
k_l^o = liquid film mass transfer coefficient without reaction,
t_e = drop exposure time,
d = drop diameter,
N_{Sh} = $k_g d/(2\ P\ Dl)$,
D_l = liquid diffusion coefficient,
Φ = $4Dl\ t_e/d^2$,
a_n = nth root of $a_n \cot(a_n) + (N_{sh}-1) = 0$,
h = drop fall height, and
v_g = terminal settling velocity of the drop.

Equations 4 and 8 result in a washout rate constant:

$$\lambda = \frac{6\ k_g F\ h}{V\ v_g\ d}\ . \tag{8}$$

Using this equation for the removal rate constant, the equation for the concentration in the gas is:

$$C = C_o\ \exp\left(\frac{-6\ k_g\ F\ h\ t}{V\ v_g\ d}\right). \tag{9}$$

The property P is referred to as an "effective" partition coefficient because it relates the total concentration of species containing iodine, I^-, in the liquid to the gas phase at the interface. The

"effective" partition coefficient for aqueous iodine is defined as:

$$P = \frac{[I_2\ (liquid)] + [I_2(reacted)]}{[I_2\ (gas)]}\ , \qquad (10)$$

where the square brackets represent the concentration of the species.

A model often used today referred to as the "realistic" model[2] is the well-mixed drop model with a partition coefficient of 100,000; this appears to give satisfactory results (see Figure 2 for comparison to existing data). The major problems with the "realistic" model are that it does not describe the iodine hydrolysis reactions, it does not deal with the liquid phase concentration, and it uses an effective partition coefficient. The effective partition coefficient is that it lumps the effects of the reactions into a single constant. The effects of the kinetics on the rate of mass transfer, under all conditions, are not constant (see Chapter 3). The temperature of the spray solution, the initial concentration of the spray solution, the pH of the spray solution, and the contact time of the individual drops all will significantly affect the rate of mass transfer. Therefore, a different effective partition coefficient is required for each condition which might

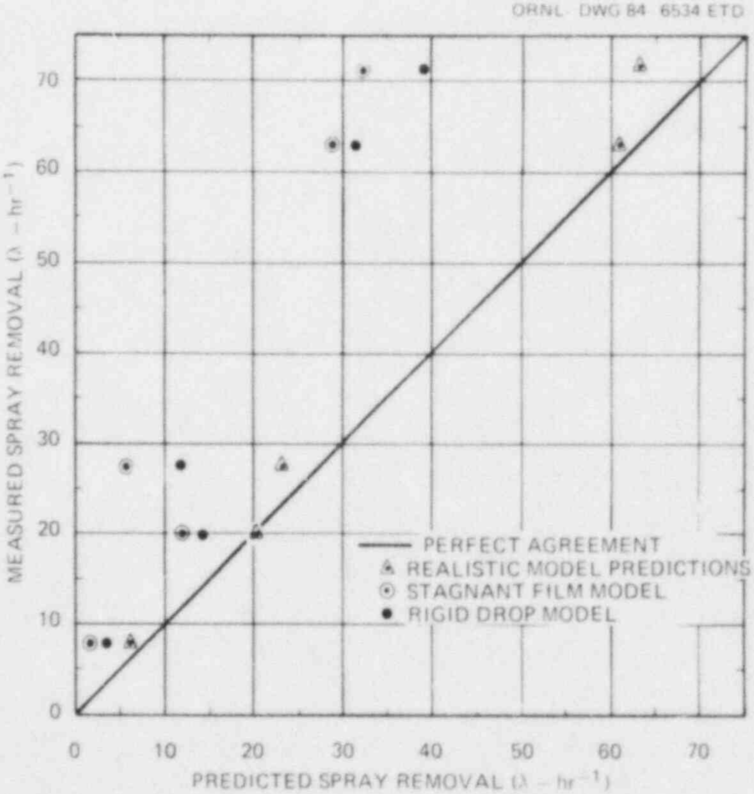

Fig. 2. Comparison of Iodine Washout Predicted by Several Models with that Measured in CSE Using Caustic Spray.[3]

exist. For these reasons, the "realistic" model will predict the same removal rate for an initial concentration in the liquid of moleclar iodine of zero and for an initial concentration in the liquid near equilibrium.

The best available experimental results that might be used in an effort to judge the efficacy of the "realistic" model are the results obtained in the Containment Systems Experiments (CSE) which are discussed in Chapter 7.[3] Briefly, these experiments are large scale containment system tests in which one of the goals of the tests was to determine the rate of removal of gaseous molecular iodine by water sprays. Some of the experimental runs used recirculatory sprays. For example, the third spray period of run A-4 (see Figure 55) is a recirculatory spray. The data show desorption of iodine from the spray solution. The so-called "realistic" model would predict that iodine is still being removed from the gas phase.

2. MASS TRANSFER

2.1 General Mass Transfer with Reaction

Mass transfer between two phases occurs because of a chemical potential driving force between the bulk of each phase and the interface.[4] When the chemical potential driving force is greater in the gas phase than in the liquid phase (see Figure 3), the component being absorbed diffuses through the gas film to the interface of the drop where equilibrium is achieved. This phenomena is usually referred to as the "gas-film resistance", which suggests a stagnant gas film of finite thickness through which the soluble gas is transferred by molecular diffusion.[5] The transferring species then diffuses from the liquid interphase to the bulk of the liquid. A concentration gradient exists in the liquid phase, just as in the gas phase, and this is referred to as the "liquid-film resistance", suggesting a stagnant liquid film of finite thickness at the interface. The bulk liquid may be completely mixed and thus have a uniform concentration, or it might be stagnant with the concentration of the transferring species decreasing as the distance from the interface increases, or the bulk liquid could be partially mixed. When chemical reactions occur in the bulk liquid, the concentration of the diffusing species can be reduced (or even eliminated) by the reactions. This can give a higher driving force due to the lower concentration of the transferring species in the bulk liquid.

Complications can occur when determining the effect of the chemical reactions on the mass transfer rate. As the transferring species diffuses through the liquid, that species is partially or possibly totally removed from the liquid by the chemical reactions. The rate of mass transfer may be increased further because the concentration gradient driving force at the interface becomes steeper (see Astarita[4] or

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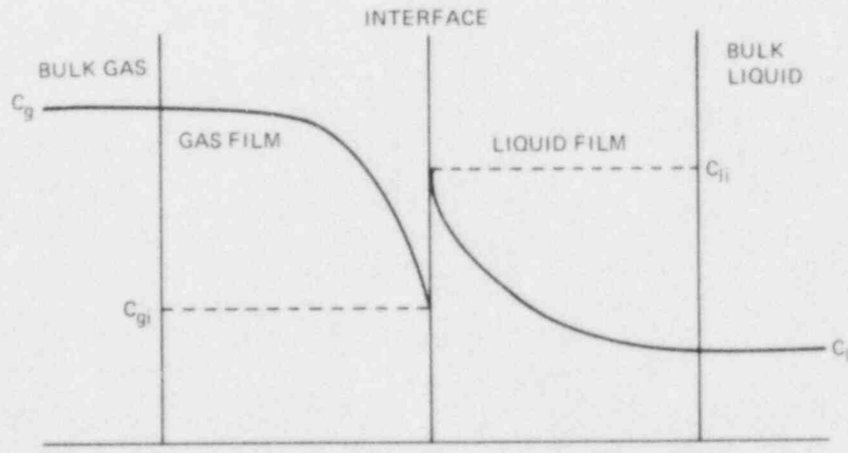

Fig. 3. Concentration Profiles for the Two Resistance Models.

Dankwerts[5] for more details). On the other hand, if the reaction in the liquid occurs very slowly, it might not affect the rate of mass transfer. A fast reaction in the liquid will increase the rate of mass transfer to a greater extent by removing the diffusing species from within the liquid film. A instantaneous reaction that occurs on the surface completely eliminates the contribution of the liquid phase to the rate of mass transfer.

The unsteady-state differential equation for diffusion with simultaneous reaction of the diffusing species is:[4]

$$D\, \Delta_2 C = u \cdot \nabla C + \partial C/\partial t + R \,. \tag{11}$$

These terms represent the relation

molecular transport = convection + accumulation + reaction rate,

where

Δ_2 = Laplacian operator = $\partial^2/\partial x_1^2 + \partial^2/\partial x_2^2 + \partial^2/\partial x_3^2$,
∇ = Nabla operator = $\sigma_1\, \partial/\partial x_1 + \sigma_2\, \partial/\partial x_2 + \sigma_3\, \partial/\partial x_3$,
u = velocity <vector>,
C = concentration of the diffusing species,
t = time, and
R = reaction rate.

For the penetration theory in one-dimension in spherical coordinates, this equation reduces to:[4]

$$D_1\left(\frac{\partial^2 C}{\partial r^2} + \frac{2}{r}\frac{\partial C}{\partial r}\right) = \frac{\partial C}{\partial t} + R \,. \tag{12}$$

Where r is the distance from the outer radius of the drop.
For the film theory (which assumes steady state in the film) in one-dimension, the unsteady-state diffusion equation reduces to

$$D_1\left(\frac{\partial^2 C}{\partial r^2} + \frac{2}{r}\frac{\partial C}{\partial r}\right) = R \,. \tag{13}$$

These equations can be solved analytically for simple kinetics. In general, the solution involves solving a series of differential equations for all species present.[5] For the complex differential equations resulting from the iodine hydrolysis reactions (see Chapter 3), an analytical solution for the unsteady-state diffusion equation with reaction is not possible, and a numerical solution is required.

2.2 Overall Mass Transfer Resistance for Iodine Absorption into Water Droplets

When mass transfer occurs between two phases, the resistance to diffusion of both phases will influence the rate of mass transfer. If one phase's contribution to the overall resistance is much smaller than the contribution of the other phase, the effect of the phase, with the smaller resistance, may be ignored because it will not significantly affect the overall rate of mass transfer. The overall mass transfer resistance is the sum of the two resistances. For a soluble gas transported across both films, one can write for a completely mixed drop:[6]

$$M_r = k_g (C_g - C_{gi}) = k_l^o (C_{li} - C_l) \tag{14}$$

where

M_r = rate of mass transfer,
k_g = gas-side mass transfer coefficient,
k_l^o = liquid-side mass transfer coefficient with no reactions,
C_g = concentration in the bulk gas,
C_{gi} = concentration in the gas at the interface,
C_l = concentration in the bulk liquid, and
C_{li} = concentration in the liquid at the interface.

Using a partition coefficient $P = C_{li}/C_{gi}$:

$$M_r = k_g (C_g - C_{gi}) = k_l^o (P\, C_{gi} - C_l) \tag{15}$$

Solving for C_{gi}:

$$k_g (C_g - C_{gi}) = k_l^o (P\, C_{gi} - C_l) \tag{16}$$

$$C_{gi} = \frac{k_l^o C_l + k_g C_g}{k_g + k_l^o P} \, . \tag{17}$$

Substituting into Equation 15, one obtains:

$$M_r = \frac{(P\ C_g - C_l)}{[1/(k_l^o) + P/k_g]} = K_{lov}\ (P\ C_g - C_l) \tag{18}$$

where

$$K_{lov} = \frac{1}{1/k_l^o + P/k_g}\ , \tag{19}$$

where K_{lov} is the overall liquid-side mass transfer coefficient.

To estimate the relative contribution of the individual resistances (for the case of completely mixed bulk liquid and no chemical reactions), one can calculate the overall mass transfer coefficient and compare with the reciprocal of the individual gas and liquid mass transfer coefficients. (See Chapter 4, DROP MODEL, for calculation equations for mass transfer coefficients.) At 25°C:

$$k_g = 10.75 \text{ cm/sec},$$

$$k_l^o = 0.25 \text{ cm/sec},$$

$$P = 86.8,$$

$$\frac{1}{K_{lov}} = \frac{1}{0.25} + \frac{86.8}{10.75}\ , \text{ and}$$

$$K_{lov} = 0.0826 \text{ cm/sec}.$$

This indicates that there is significant resistance to mass transfer in both phases when no reactions occur. The chemical reactions that occur in the liquid (see Chapter 3, AQUEOUS IODINE CHEMISTRY) will tend to decrease the significance of the liquid phase.

3. AQUEOUS IODINE CHEMISTRY

The chemistry of aqueous iodine has been studied in depth by Bell,[7] Sellers,[8] and Eigen.[9] The true reaction mechanisms of iodine and water are not known. The following reactions involving iodine and water are the best equation available for a mass transfer with reaction model:[9]

$$1)\quad I_2 + H_2O \underset{k_{-1}}{\overset{k_1}{\rightleftarrows}} HOI + I^- + H^+ , \tag{20}$$

$$2)\quad 3HOI \underset{k_{-2}}{\overset{k_{20},\ k_{21}}{\rightleftarrows}} IO_3^- + 2I^- + 3H^+ , \tag{21}$$

$$3)\quad 4I^- + O_2 + 4H^+ \overset{k_3}{\rightarrow} 2I_2 + 2H_2O , \tag{22}$$

$$4)\quad I_2 + I^- \underset{k_{-4}}{\overset{k_4}{\rightleftarrows}} I_3^- , \tag{23}$$

$$5)\quad HOI \underset{k_{-5}}{\overset{k_5}{\rightleftarrows}} H^+ + OI^- , \tag{24}$$

$$6)\quad H_2O \underset{k_{-6}}{\overset{k_6}{\rightleftarrows}} H^+ + OH^- . \tag{25}$$

Note that this treatment essentially considers iodine hydrolyses as a two step mechanism given by equations 20 and 21. The other equations give terms related to this assumed two step process.

The kinetic rate equations developed for the chemical equations above are:

$$d[I_2]/dt = -k_1[I_2] + k_{-1}[I^-][HOI][H^+] + 0.5\ k_3[H^+][O_2][I^-] - k_4[I_2][I^-] , \tag{26}$$

$$d[I^-]/dt = k_1[I_2] - k_{-1}[I^-][HOI][H^+] + (2/3)\ k_{20}[HOI]^2 + (2/3)\ k_{21}[HOI][OI^-] - 2\ k_{-2}[IO_3^-][I^-]^2[H^+]^2 - k_3\ [H^+][O_2][I^-] - k_4[I_2][I^-] , \tag{27}$$

$$d[HOI]/dt = k_1\ [I_2] - k_{-1}[I^-][HOI][H^+] - k_{20}\ [HOI]^2 - k_{21}[HOI][OI^-] + 3\ k_{-2}[IO_3^-][I^-]^2[H^+]^2\ , \tag{28}$$

$$d[IO_3^-]/dt = (1/3)\ k_{20}[HOI]^2 + (1/3)\ k_{21}[HOI][OI^-] - k_{-2}[IO_3^-][I^-]^2[H^+]^2\ , \tag{29}$$

$$d[I_3^-]/dt = k_4[I_2][I^-] - k_{-4}[I_3^-] + k_3[H^+][O_2][I^-]\ , \tag{30}$$

$$d[H^+]/dt = k_1[I_2] - k_{-1}[I^-][HOI][H^+] + k_{20}[HOI]^2 + k_{21}[HOI][OI^-] - 3\ k_{-2}[IO_3^-][I^-]^2[H^+]^2 - k_3[H^+][O_2][I^-]\ . \tag{31}$$

The stoichiometry of Equations 20 through 25 are not represented in the Equations 26 through 30 because Equations 26 through 30 are derived from experimental observations.[7] Equation 31 was derived by incorporating the individual rate expressions used by Bell.[7]

The first reaction has been assigned a pseudo first order rate constant for the forward reaction and a third order rate constant has been assigned to the reverse reaction. This reaction is fast and comes to equilibrium in a few seconds (see Table 1 for rate constants). There is a pH dependency since hydrogen ions (H^+) are formed and the extent of the reaction varies greatly with the pH of the solution. The existence of hypoiodous acid, HOI, has not been proven; however, HOI is thought to be formed.[7]

The second reaction has been assigned a two term rate equation in which both expressions have a second order rate constant for the forward reaction and a fifth order rate constant for the reverse reaction. The second reaction is much slower than the first reaction and comes to equilibrium in a period of time varying from approximately fifteen seconds to well over one year depending on the pH. As in the first reaction, the higher the pH, the faster the reaction rate.

The third reaction is irreversible. The concentration of oxygen is assumed to be constant and is related to the concentration of oxygen in the gas by a Henry's coefficient. A pseudo second order rate constant k_{p3}, can then be assigned to this reaction.[7]

$$k_{p_3} = k_3\ [O_2] \tag{32}$$

In this third reaction, molecular iodine is a product, and the reaction is also pH dependent. At a low pH, the equilibrium shifts to the right, resulting in the production of more molecular iodine. But the production of molecular iodine by this reaction is small. Therefore, the

Table 1. Values of rate of equilibrium constants (Bell[7])

Constant	Temperature (°C)	Value
k_1[a]	20	$3\ s^{-1}$
k_{-1}	20	$4.4 \times 10^{12}\ \underline{M}^{-2}\ s^{-1}$
k_{20}	25	$250\ \underline{M}^{-1}\ s^{-1}$
k_{21}	25	$120\ \underline{M}^{-1}\ s^{-1}$
k_{-2}	25	$3 \times 10^{8}\ \underline{M}^{-4}\ s^{-1}$
k_3	25	$3.475 \times 10^{-4}\ \underline{M}^{-2}\ s^{-1}$
k_4	25	$3 \times 10^{6}\ \underline{M}^{-1}\ s^{-1}$
k_{-4}	25	$4 \times 10^{3}\ s^{-1}$
K_4	25	736
K_5	25	2.3×10^{-11}
K_6	25	1.006×10^{-14}

[a]The value of k_1 was calculated by Eigen and Kustin,[9] who assumed that $K_1 = 6.8 \times 10^{-13}\ \underline{M}^2$.

third reaction also produces more beneficial effects, at a high pH, by producing molecular iodine than at a low pH.

Reaction four involves the formation of tri-iodide. This reaction is very important because it is essentially instantaneous and removes molecular iodine from the solution. A second order rate constant is assigned to the forward reaction and a first order rate constant is assigned to the reverse reaction.[7]

Reaction five is the dissociation of hypoiodous acid, and reaction six is the dissociation of water. Both reaction five and six are essentially instantaneous.

The most important reactions are the first and the fourth reactions. Both of these reactions remove molecular iodine from the solution, and by lowering the concentration of molecular iodine, the concentration driving force for mass transfer increases.

The most important species besides molecular iodine is the hydrogen ion concentration. Overall, the removal of molecular iodine from solution is increased when the pH of the solution is high and is decreased when the pH is low. All of the reactions except reaction four contain terms involving the hydrogen ion concentration.

At a high pH, the combined result of all reactions is to deplete the concentration of molecular iodine in solution. As a result, the

concentration driving force for mass transfer is increased, and the mass transfer rate is increased. It is also very desirable to have the pH buffered because sufficient hydrogen ions are produced that otherwise would cause the pH to drop very quickly to a point where the reactions would essentially stop.

Little information is available concerning the temperature dependencies of these reactions. For reactions 1 through 3, no experimental information is available for the temperature dependencies. The temperature dependence upon the equilibrium constants for reactions 4 through 6 are:[7]

$$\text{Ln } K_4 = 3727.86/T - 11.6326 + 0.0192212\ T \tag{33}$$

$$\text{Log } K_5 = 2800.48 + 0.7335\ T - 80670./T - 1115.1\ (\text{Log } T) \tag{34}$$

$$\text{Log } K_6 = -4.098 - 3245.2/T + 2.2367 \times 10^5/T^2 - 3.984 \times 10^7/T^3 + (13.957 - 1262.3/T + 8.5641 \times 10^5/T^2)\ \text{Log DENLIQ} \tag{35}$$

where DENLIQ, the density of water which was derived by a numerical fit to experimental data,[10] is given by:

$$\text{DENLIQ} = 6.0251147 \times 10^{-9}\ T^3 - 9.1329064 \times 10^{-6}\ T^2 + 3.573572 \times 10^{-3}\ T + 5.835882 \times 10^{-1} \text{, and} \tag{36}$$

T = temperature, K.

A numerical model which simulates the iodine hydrolysis reactions has been developed (see Appendix B). The model uses a Runge-Kutta-Felhburg (RKF) algorithm[11] which numerically integrates the kinetic rate equations 26 through 31 as a function of time. Figure 4 shows the algorithm for the kinetic model. Inputs to the model are:

1) temperature of the solution,
2) initial concentration of all species in the solution,
3) whether buffered or unbuffered (see Appendix A, Numerical Technique), and
4) simulation time.

Output from the model produces one file and one plot. File FOR50.DAT contains the concentration of all species as a function of time (see Appendix B for a sample output). This file is used to make a plot of concentration of all species in the liquid versus time.

Figures 5 through 13 show the chemical kinetics as a function of time for initial concentrations of molecular iodine of 1.0×10^{-3} to 1.0×10^{-10} moles/liter and the initial concentration of the other species

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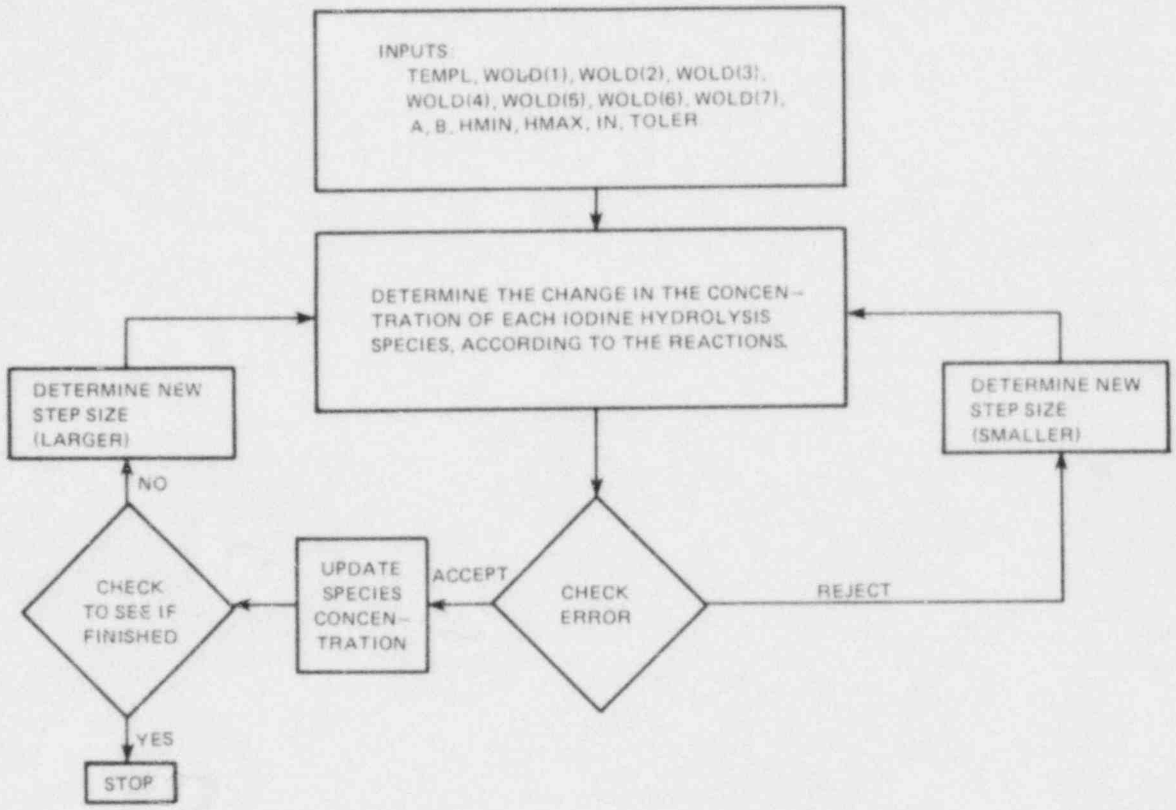

Fig. 4. Kinetic Model Flowsheet.

were zero. These plots were produced by numerically integrating the iodine hydrolysis reactions (see Appendix A for a description of the numerical technique). The fifteen-second time scale was chosen as the maximum drop lifetime because fifteen-seconds is the maximum time a drop would experience in a containment safety spray system (for longer reaction times see Reference 7).

These plots show that the concentration of molecular iodine decreases as the conversion of molecular iodine increases. For example, with an initial concentration of molecular iodine of 1×10^{-3} moles/liter and with a buffered pH of 9.0, Figure 5a, the equilibrium concentration of molecular iodine is by a factor of approximately five less than the initial concentration. At an initial concentration of molecular iodine of 1×10^{-10} moles/liter and a buffered pH of 9.0, Figure 12a, the equilibrium concentration of molecular iodine is almost seven orders of magnitude less than the initial concentration. The leveling-off of the change in the concentration of molecular iodine that occurs before 5 seconds is due mainly to the equilibration of the first reaction. The effects of the second reaction are not as obvious, but after the plateau has occurred, the concentration of molecular iodine is still dropping and the concentration of iodide, I^-, is increasing due to the second reaction. The second reaction equilibrates very slowly and this equilibrium is shown in the figures provided by Reference 7.

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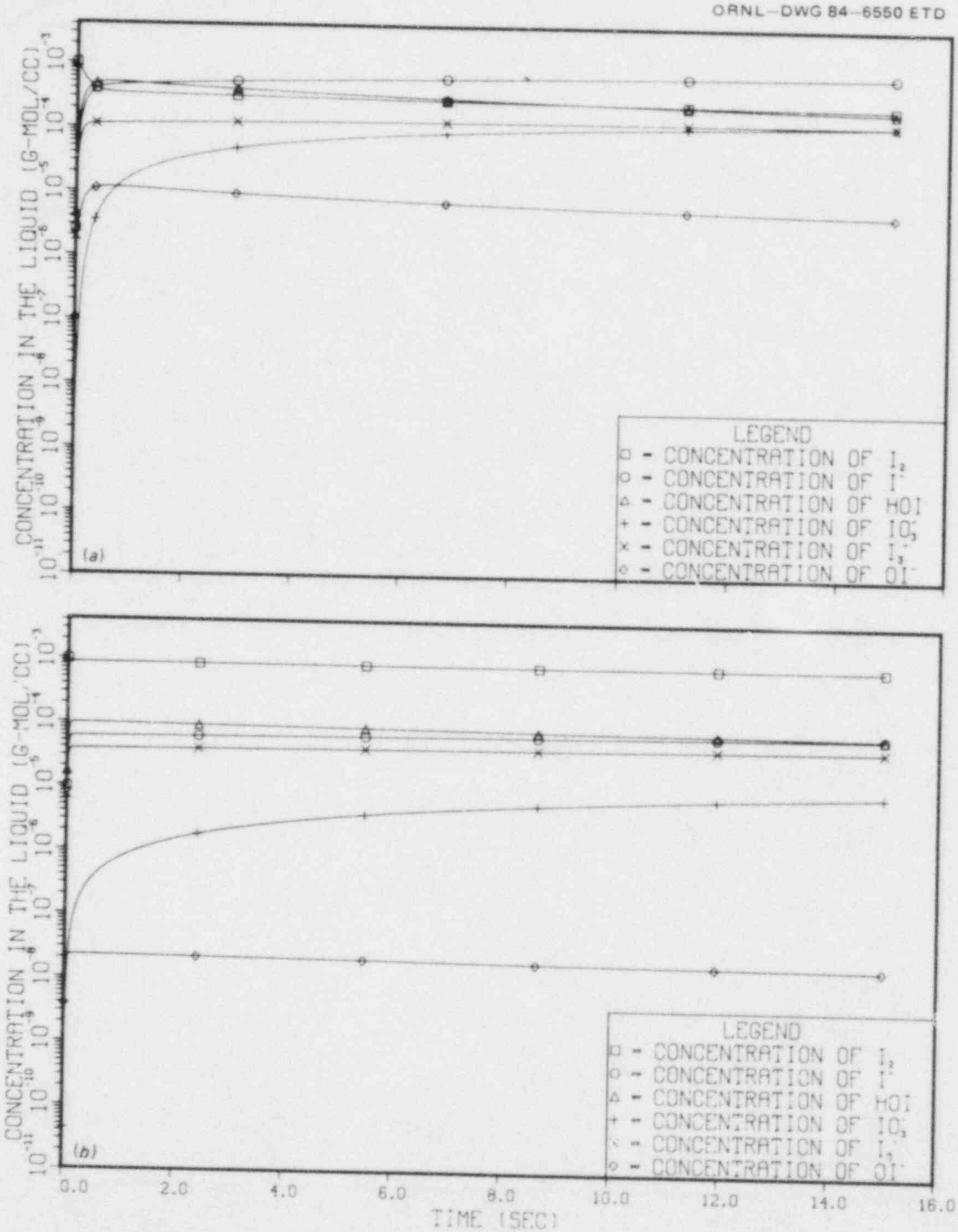

Fig. 5. Results of Kinetic Model. Initial concentration of molecular iodine 1.0×10^{-3} moles/liter.
(a) Buffered pH of 9.0.
(b) Buffered pH of 7.0.

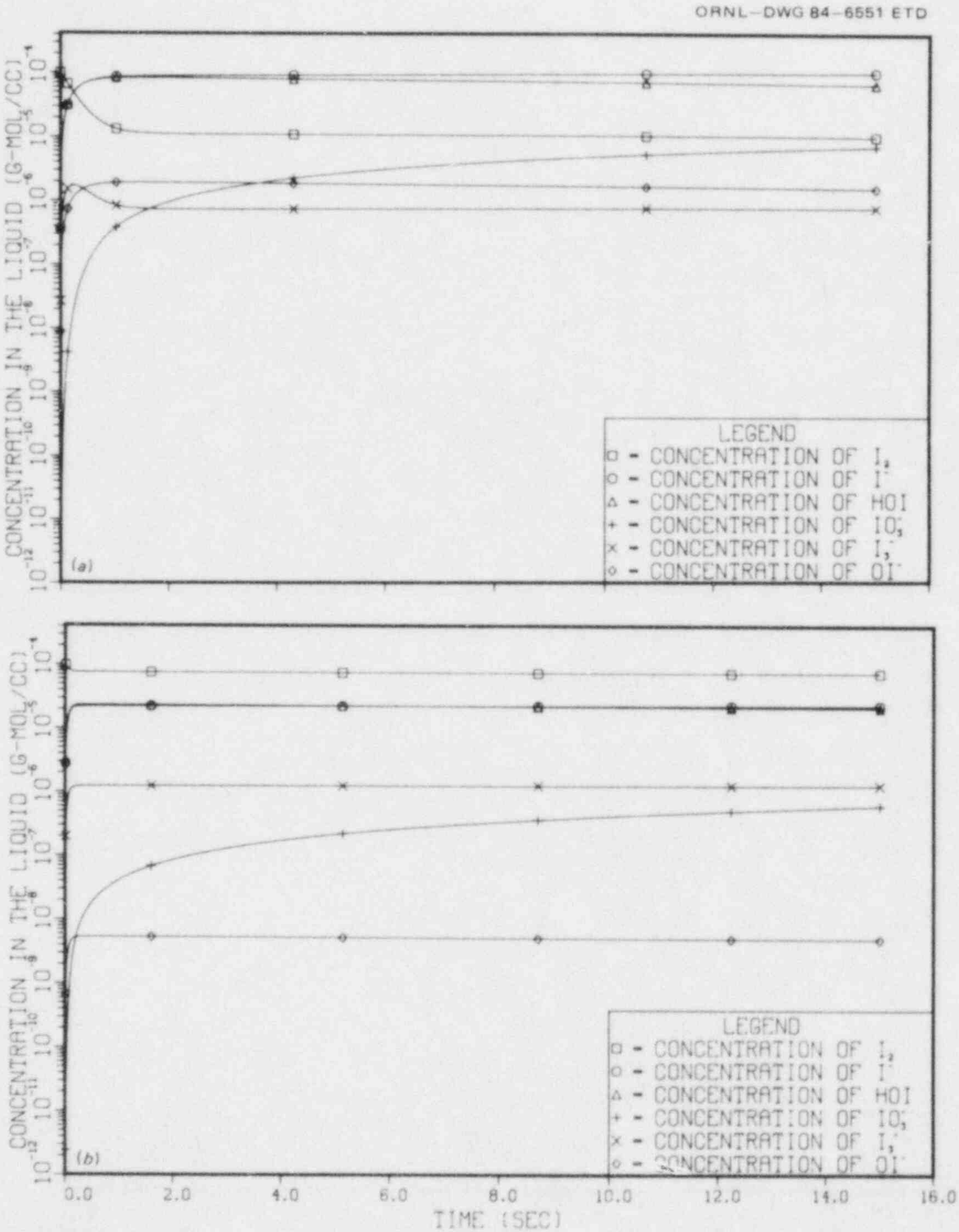

Fig. 6. Results of Kinetic Model. Initial concentration of molecular iodine 1.0×10^{-4} moles/liter.
(a) Buffered pH of 9.0.
(b) Buffered pH of 7.0.

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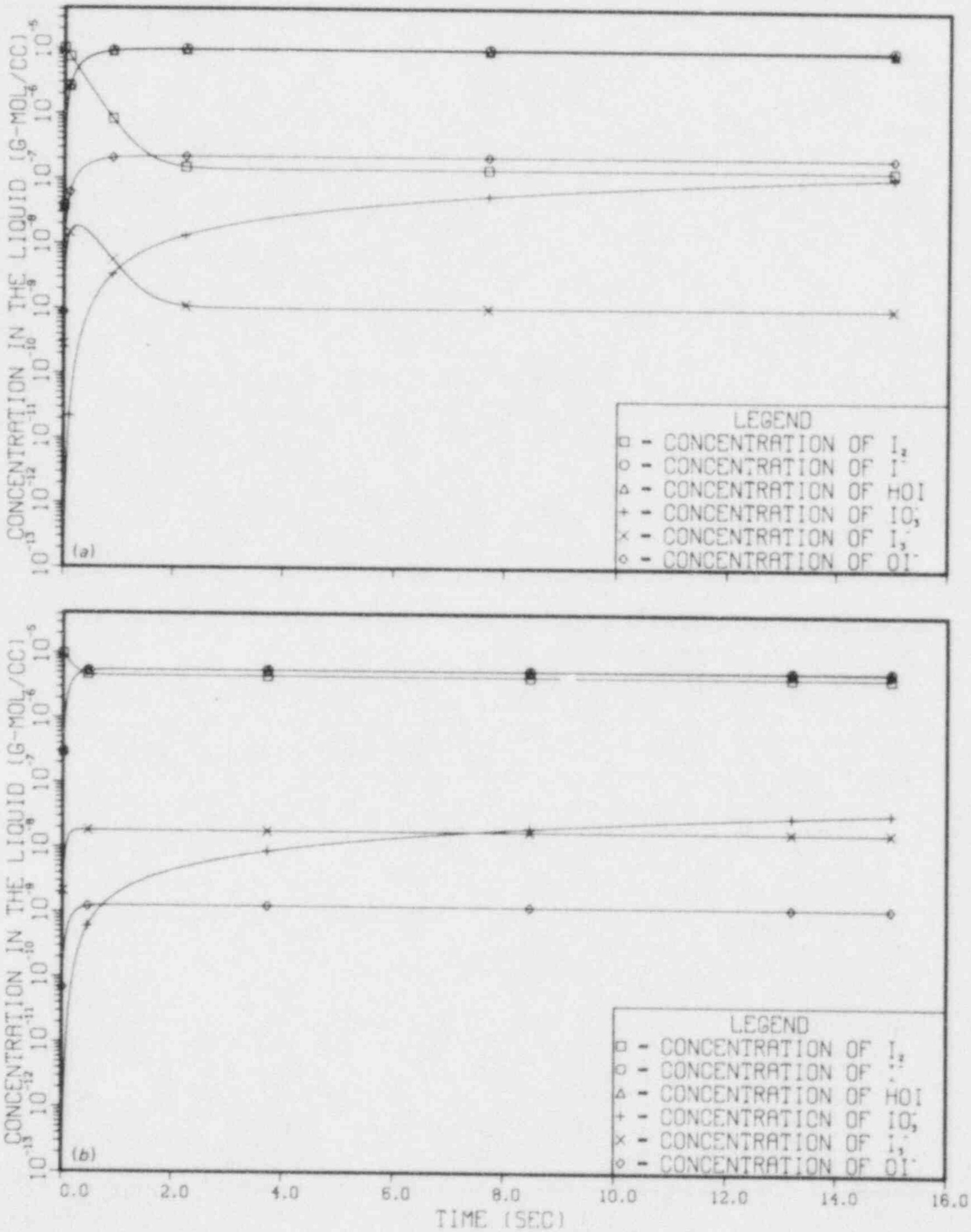

Fig. 7. Results of Kinetic Model. Initial concentration of molecular iodine 1.0×10^{-5} moles/liter.
(a) Buffered pH of 9.0.
(b) Buffered pH of 7.0.

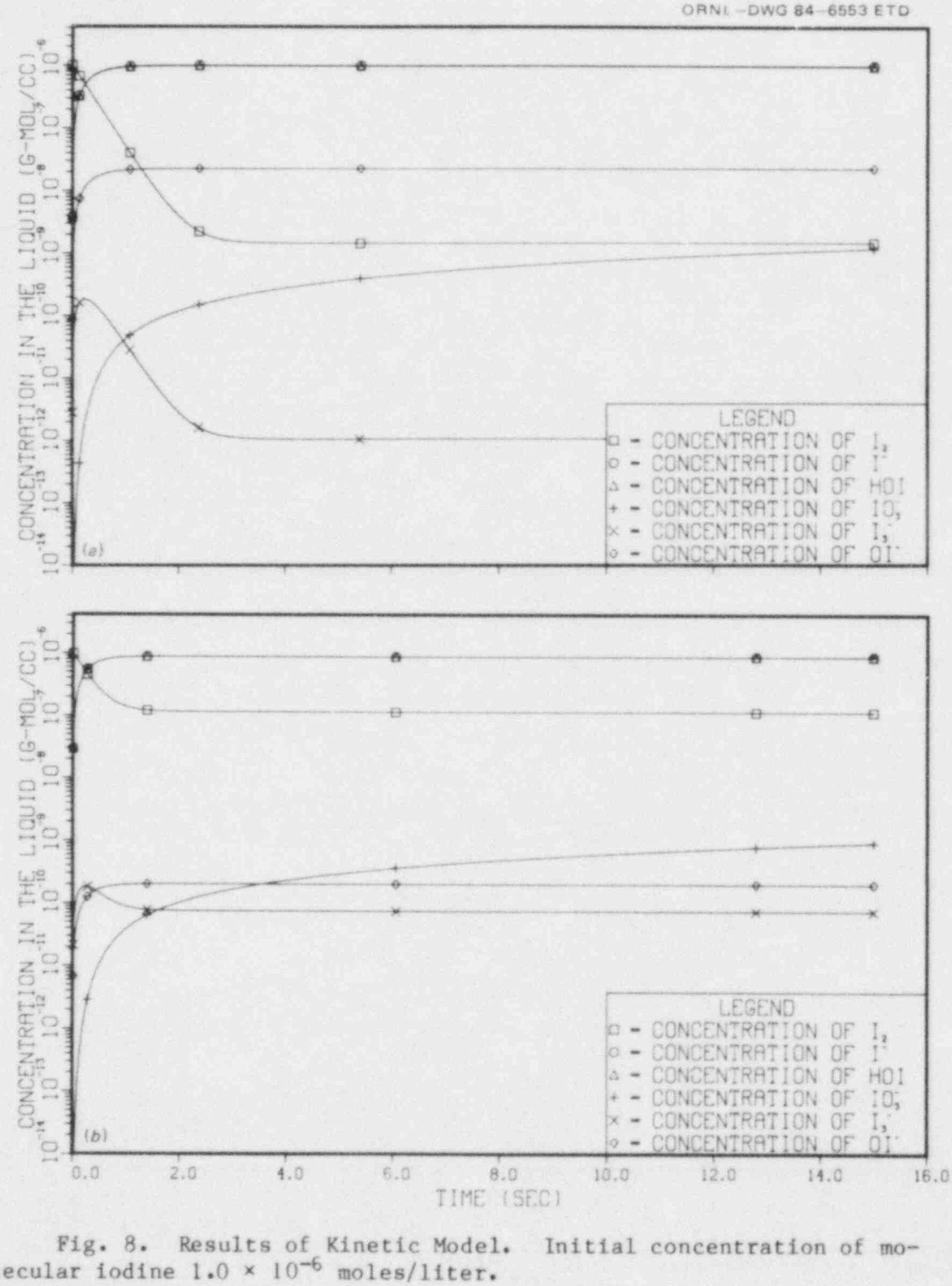

Fig. 8. Results of Kinetic Model. Initial concentration of molecular iodine 1.0×10^{-6} moles/liter.
(a) Buffered pH of 9.0.
(b) Buffered pH of 7.0.

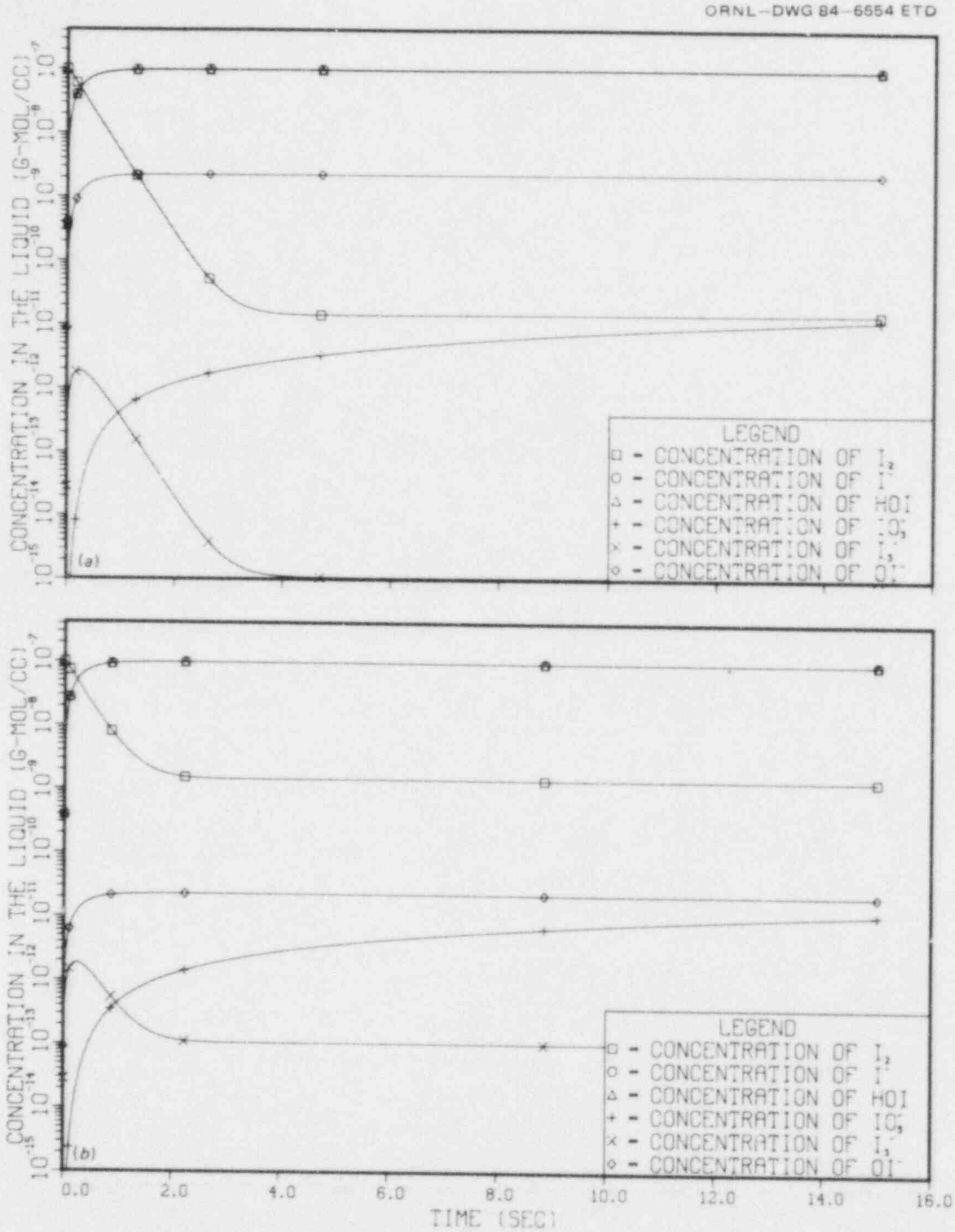

Fig. 9. Results of Kinetic Model. Initial concentration of molecular iodine 1.0×10^{-7} moles/liter.
(a) Buffered pH of 9.0.
(b) Buffered pH of 7.0.

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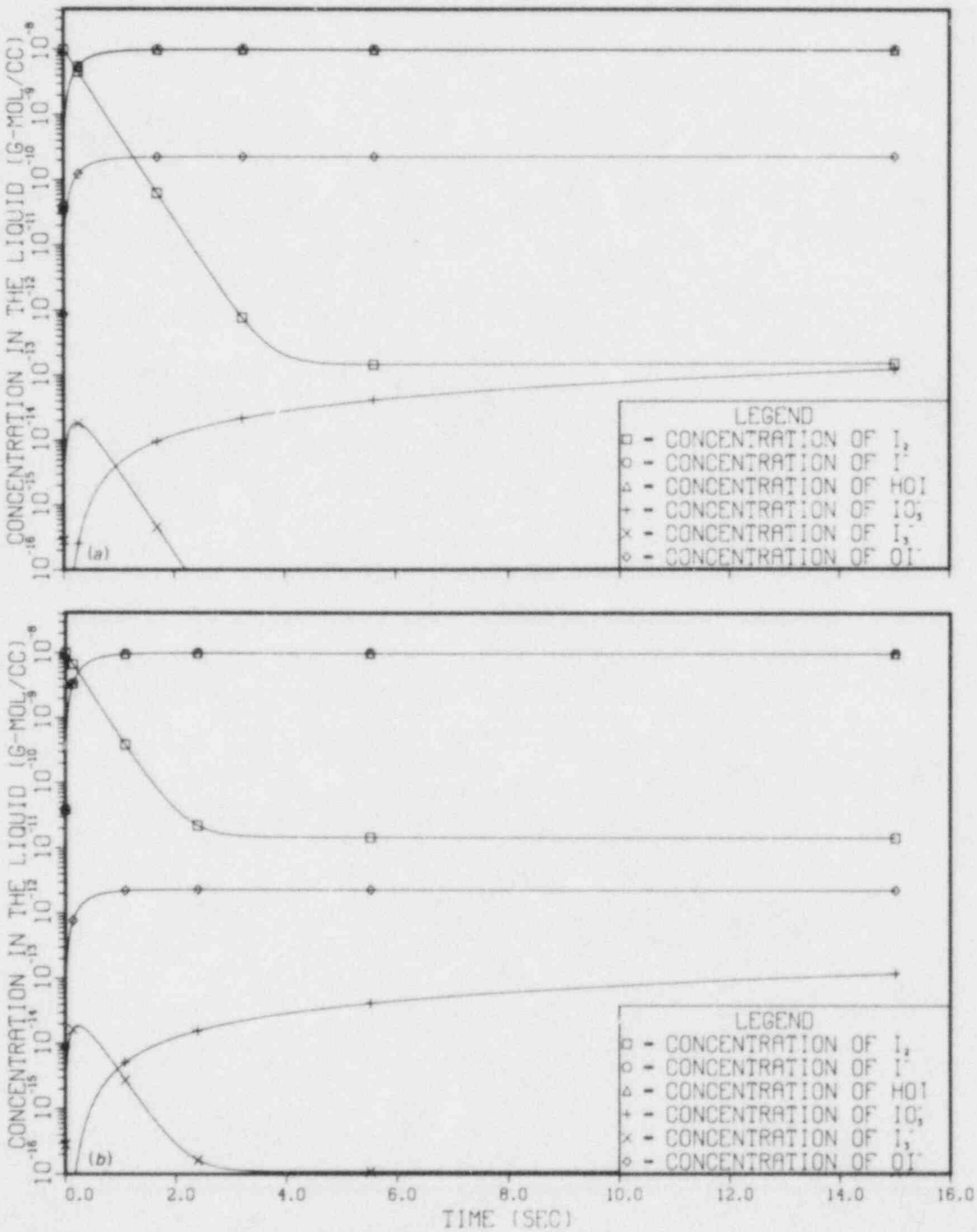

Fig. 10. Results of Kinetic Model. Initial concentration of molecular iodine 1.0×10^{-8} moles/liter.
(a) Buffered pH of 9.0.
(b) Buffered pH of 7.0.

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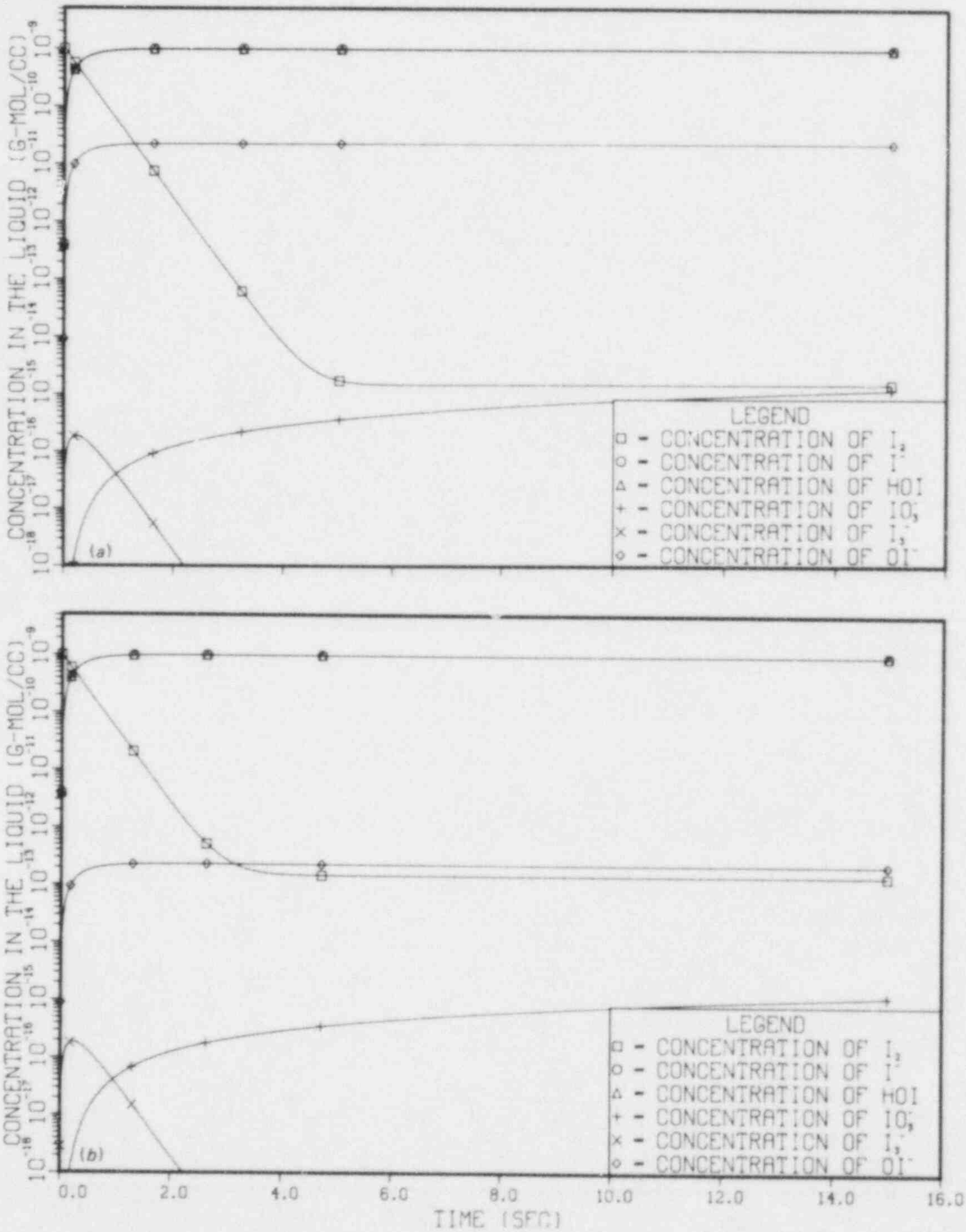

Fig. 11. Results of Kinetic Model. Initial concentration of molecular iodine 1.0×10^{-9} moles/liter.
(a) Buffered pH of 9.0.
(b) Buffered pH of 7.0.

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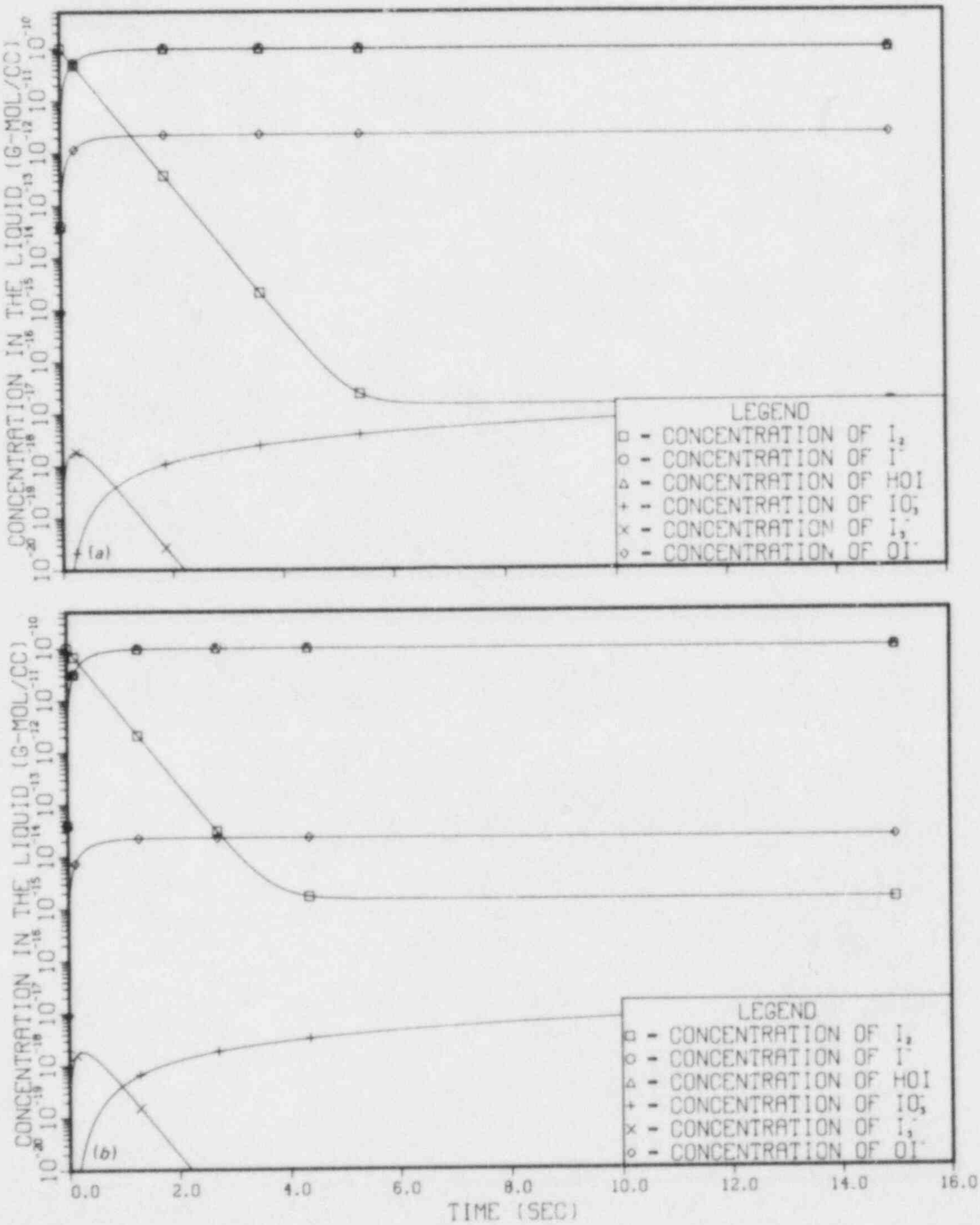

Fig. 12. Results of Kinetic Model. Initial concentration of molecular iodine 1.0×10^{-10} moles/liter.
(a) Buffered pH of 9.0.
(b) Buffered pH of 7.0.

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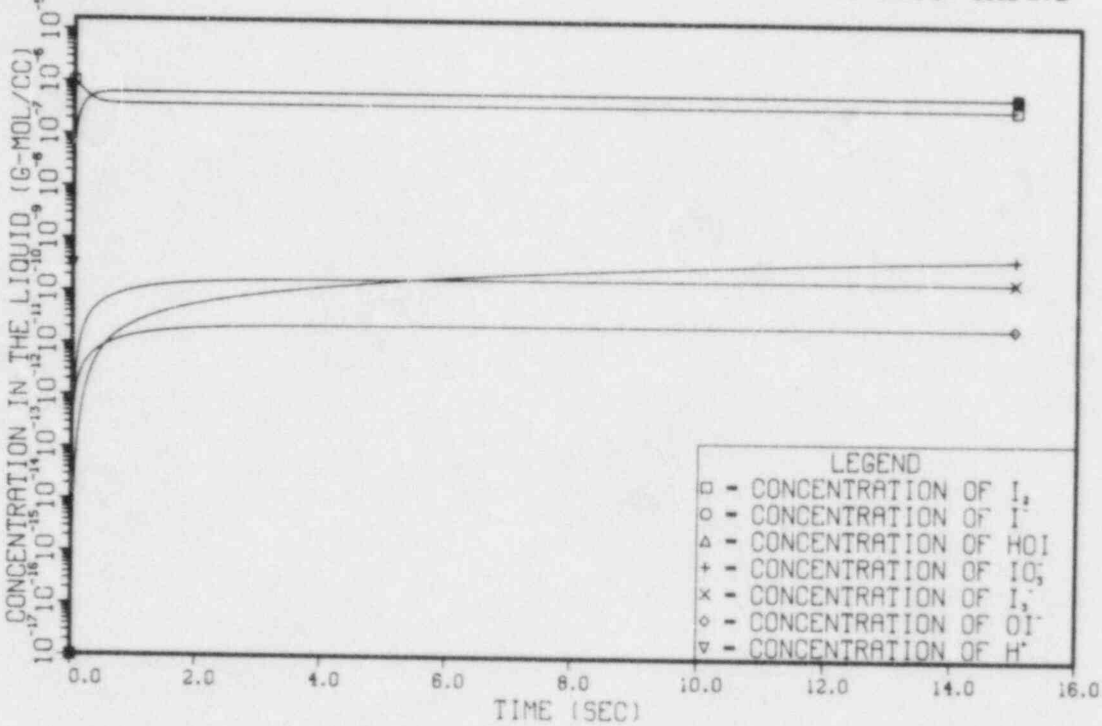

Fig. 13. Results of Kinetic Model. Initial concentration of molecular iodine 1.0×10^{-6} moles/liter Unbuffered pH of 9.5.

In Figures 5 through 12, part a is for a buffered pH of 9 in the liquid while part b presents the results for a buffered pH of 7. Comparing the two parts, the conversion of molecular iodine for the same initial concentration is much greater for the pH 9 solutions than for the pH 7 solutions. For a pH of 7 and a high concentration of molecular iodine (above 1.0×10^{-7} moles/liter), the fraction of molecular iodine conversed is small but as the initial concentration of molecular iodine decreases, the conversion of molecular iodine increases. At an initial concentration of molecular iodine of 1.0×10^{-10} moles/liter, the concentration of molecular iodine, at equilibrium, decreases by five orders of magnitude for a buffered pH of 7.0 as opposed to a decrease of 7 orders of magnitude for a buffered pH of 9.0.

Figure 13 represents results calculated for an unbuffered solution of pH 9.5 and an initial concentration of molecular iodine of 1.0×10^{-6} moles/liter. The plotted results show quite clearly the effects of the enormous quantity of hydrogen ions produced, such that the pH very quickly drops from its initial value to a pH of approximately 6, and the reactions essentially cease.

A few important conclusions can be drawn from observing the plots of the iodine hydrolysis reactions and considering their effects on the

rate of mass transfer:

1) For a solution that is buffered at a high pH, the reactions greatly increase the rate of mass transfer by decreasing the concentration of molecular iodine in the liquid. This increases the concentration driving force for mass transfer, thereby increasing the overall rate of mass transfer.
2) For a solution that is buffered at a low pH, the reactions will also increase the rate of mass transfer, but the increase will be much less than for a buffered high pH.
3) For a solution that is unbuffered at essentially any pH, the pH will almost immediately drop to a value at which reactions cease, and the reactions, therefore, will not have any substantial further effect on the rate of mass transfer.

4. DROP MODEL

The drop model simulates a single droplet suspended in gas containing molecular iodine for a specified amount of time. This model is used to calculate the rate of mass transfer for one drop and the concentration in the drop as a function of time. Water drops falling in air are essentially stagnant (non-circulating) if their diameter is less than 30 microns.[12] Drops greater than 1000 microns are significantly non-spherical, and drops break-up before they reach a diameter of 10,000 microns.[12] Safety spray systems in nuclear reactors have droplet mass medium diameters ranging from 700 microns to 1500 microns.[3] According to Clift[12] these drops are in the diameter range of non-spherical drops, with the bulk of the drop well mixed. Thus an approach was chosen such that the assumptions for the drop model are:

1) each drop has a completely mixed bulk liquid,
2) resistance to mass transfer in both the gas phase and the liquid phase,
3) molecular iodine (I_2) is the only species which transfers in or out of the drop,
4) reactions occur in the bulk of the liquid,
5) drops always fall at their terminal velocity,
6) the drop has a constant surface area and constant volume at all times,
7) the gas phase concentration is always constant (quasi-steady state), and
8) there is no transfer of heat or water between the drop and the gas phase.

The assumption of no heat transfer is made to make the model reflects only the mass transfer and the iodine hydrolysis reactions. Heat transfer will occur if there exists a temperature difference between the gas and liquid phases. Heat transfer would be important under certain conditions but consideration of it would add unnecessary complications to a completely new approach. If the results of this new approach are reasonable, then the addition of heat transfer models is the logical next step.

The drop is composed of water which may be unbuffered or buffered with a solution such as H_2BO_3 and NaOH. The presence of these solutions would not change the iodine hydrolysis reactions. The gas phase is assumed to be a mixture of air and molecular iodine (I_2). A two resistance model is used for the mass transfer rate:[6]

$$M_r = k_g (C_g - C_{gi}) \tag{37}$$

$$= k_l^o (C_{li} - C_l) \tag{38}$$

where

M_r = rate of reaction,
k_g = gas phase mass transfer coefficient,
k_l^o = liquid phase mass transfer coefficient without reaction,
C_g = concentration of molecular iodine in the gas phase,
C_{gi} = concentration of the transferring species (molecular iodine) in the gas phase at the gas-liquid interphase,
C_l = concentration of the transferring species in the liquid phase,
C_{li} = concentration of the transferring species in the liquid phase at the gas liquid interphase.

Using an overall mass transfer coefficient, the mass transfer rate may be written as:

$$M_r = K_{lov} (C_l^* - C_l) \tag{39}$$

where

K_{lov} = the overall mass transfer coefficient based on the liquid phase,
C_l^* = the equilibrium concentration of the transferring species corresponding to the interphase liquid-phase concentration,
C_l = the concentration of the transferring species in the bulk liquid,

and

$$\frac{1}{K_{lov}} = \frac{1}{k_l^o} + \frac{P}{k_g} \tag{40}$$

where P is the partition coefficient (related to a Henry's coefficient).

The gas phase mass transfer coefficient is determined by a correlation given by Clift[12] for drops in free fall in air and with diameter greater than 300 microns:

$$k_g(Sc)^{2/3} = 0.83(\Delta\rho/\rho_g)^{1/4} g^{1/4} \nu^{1/2} d^{-1/4} \tag{41}$$

where

k_g = gas phase mass transfer coefficient,
Sc = Schmidt number, $Sc = \nu/D_g$,
ν = kinematic viscosity, $\nu = \mu_g/\rho_g$,

μ_g = viscosity of the gas,

ρ_g = density of the gas,

D_g = diffusion coefficient,

$\Delta\rho$ = density of the liquid phase minus the density of the gas phase,

ρ_g = density of the gas phase,

g = acceleration of gravity, and

d = drop diameter.

This equation can be rearranged as:

$$k_g = 0.83\ (\Delta\rho/\rho_g)^{1/4} g^{1/4} (\rho_g/\mu_g)^{1/6} D_g^{\ 2/3} d^{-1/4} \qquad (42)$$

The diffusion coefficient is estimated by a binary gas system of air and molecular iodine. The mutual diffusion coefficient for a binary gas at low pressure is:[13]

$$D_g = \frac{0.001858T^{3/2}(1/Ma+1/Mb)^{1/2}}{p\ \rho_{ab}^2\ \Omega_d}\ \text{cm/sec} \qquad (43)$$

where

D_g = mutual diffusion coefficient for a binary gas,

T = temperature,

Ma = molecular weight of component a,

Mb = molecular weight of component b,

p = pressure, atm

σ_{ab} = Lennard-Jones force constant for the binary mixture, and

Ω_d = collision integral.

There are very few successful attempts to correlate the inside the drop liquid phase mass transfer coefficient. This lack of correlations could be due to the inconsistant experimental results caused by surface impurties and other experimental problems. For this study, the liquid phase mass transfer coefficient is approximated by using concepts Higbies penetration theory.

The liquid phase mass transfer coefficient is determined by Higbies penetration theory which leads to the following equation for droplets:[4]

$$k_l^o = (4\ D_l/\pi\ t^*)^{1/2} \qquad (44)$$

where

t^* = gas-liquid element contact time [for a falling liquid drop in a gas phase: $t^* = d/u$ (assumed)],
d = drop diameter,
u = velocity of drop,
π = 3.1415..., and
D_l = liquid diffusion coefficient.

Higbies penetration theory was first applied to the liquid phase mass transfer coefficients between gas bubbles and bulk water for short periods of time. As a water drop falls through air, the water inside the drop circulates causing continual renewing of the surface. Garner and Lane[14] have observed circulation within a drop as it falls in a gas. Previously reported studies[15,16] have shown appreciably greater absorption rates of a gas by water drops than predicted by theoretical rates of mass transfer in stagnant drops; the difference due to circulation within the drops. The experimental results of Garner and Lanc[14] for CO_2 absorption from a gas into liquid water drops agree reasonably well within the values used in this study based upon the Higbies penetration theory. The penetration theory is only one approach for visualizing the mass transfer resistance in a liquid film. Other theories or correlations could be used which would give slightly different values for use in these models, but the liquid side coefficients used in this study are believed to be approximately correct and representative of values observed experimentally under similar conditions.

The liquid phase diffusion coefficient is determined by Wilke and Chang:[13]

$$D_l = 7.4 \times 10^{-8}[(\Phi M_B)^{1/2}\ T/\mu_l V_A^{0.6}] \tag{45}$$

where

D_l = liquid diffusion coefficient,
V_A = 71.2 for molecular iodine,
T = temperature,
M_B = 18.015,
Φ = 2.26, and
μ_l = viscosity of the liquid.

Making these substitution, the liquid diffusion coefficient is

$$D_l = 3.653 \times 10^{-8}[T/\mu_l] \ . \tag{46}$$

The partition coefficient is determined by a fourth order numerical fit to the data presented in Table 2.[17]

Table 2. Partition coefficient of molecular iodine as a function of temperature

Temperature (K)	Molecular iodine partition coefficient
292	108.
325	29.7
359	11.6
365	10.9
424	5.1

The fourth order numerical fit to this data results in:

$$P = 9.98147 \times 10^{-7}\ T^4 - 1.5730121 \times 10^{-3}\ T^3 + 9.2785676 \times 10^{-1}\ T^2 - 2.4288388 \times 10^{2}\ T + 2.3824847 \times 10^{4} \quad (47)$$

where T is the absolute temperature, K.

The density, DENGAS, and the viscosity, VISGAS, of the gas phase are determined by a fourth order numerical fit to experimental data[10] for air. The fourth order fit for the density of the gas is:

$$DENGAS = 8.2892005 \times 10^{-16}\ T^4 - 4.2656962 \times 10^{-12}\ T^3 + 8.0228283 \times 10^{-9}\ T^2 - 6.8325529 \times 10^{-6}\ T + 2.6129391 \times 10^{-3}\ \text{gm/cc}\ , \quad (48)$$

where T is in K. The viscosity of the gas in centipoise is expressed by:

$$VISGAS = -2.8713193 \times 10^{-15}\ T^4 + 1.6909463 \times 10^{-11}\ T^3 - 4.015468 \times 10^{-8}\ T^2 + 6.5679429 \times 10^{-5}\ T + 1.9523691 \times 10^{-3}\ , \quad (49)$$

where T is in K.

The viscosity of the liquid, VISLIQ, is determined by a fourth order numerical fit to experimental data for water.[18] The expression for the viscosity in centipoise is:

$$\begin{aligned} \text{VISLIQ} = {} & 1.8662866 \times 10^{-8}\ T^4 - 2.633395 \times 10^{-5}\ T^3 \\ & + 1.3970607 \times 10^{-2}\ T^2 - 3.3074806\ T \\ & + 2.9558666 \times 10^{2}\ , \end{aligned} \tag{50}$$

where T is in K.

The density of the liquid, DENLIQ, is determined by a third order fit to experimental data for water.[18] The numerical fit results in

$$\begin{aligned} \text{DENLIQ} = {} & 6.0251147 \times 10^{-9}\ T^3 - 9.1329604 \times 10^{-6}\ T^2 \\ & + 3.573572 \times 10^{-3}\ T + 5.835882 \times 10^{-1}\ \text{gm/cc}\ , \end{aligned} \tag{51}$$

where T is in K.

The Reynolds number of the drop is determined by a correlation by Clift.[12] The first step is:

$$N_D = 4\ \rho_g \Delta\rho\ g\ d^3/3\mu_g{}^2 \tag{52}$$

where

N_D = "Best Number" ($3N_D/4$ is called Galileo number or Archimedes number),
ρ_g = density of the gas,
$\Delta\rho$ = (density of the liquid — density of the gas),
g = acceleration of gravity,
d = diameter of the drop, and
μ_g = viscosity of the gas.

The Reynolds number can then be calculated by:

$$\begin{aligned} \text{Log}_{10}(N_{Re}) = {} & -1.81391 + 1.34671\ \text{Log}_{10}\ N_D - 0.12427\ (\text{Log}_{10}N_D)^2 \\ & + 0.006344\ (\text{Log}_{10}N_D)^3\ , \end{aligned} \tag{53}$$

where N_{Re} is the drop Reynolds number .

The terminal velocity, TRMVEL, can then be determined from the drop Reynolds number:

$$TRMVEL = N_{Re}\ \mu_g / d\ \rho_g \tag{54}$$

where

μ_g = viscosity of the gas, and
ρ_g = density of the gas.

The exposure time, EXPTM, can then be determined by:

$$EXPTM = HEIGHT/TRMVEL\ , \tag{55}$$

where HEIGHT is the drop fall height.

The drop model is a quasi-steady state algorithm (see Figure 14 for DROP MODEL flowsheet). The algorithm is:

1) determine the number of moles of molecular iodine that are transferred to the drop from the gas phase,
2) calculate the concentration of molecular iodine in the liquid drop,
3) determine the concentration of all species in the liquid drop due to the iodine hydrolysis reactions, and
4) loop back to 1) until droplet fall time is reached.

The input parameters for the drop model are:

1) initial gas phase concentration of molecular iodine,
2) initial liquid phase concentration of all iodine hydrolysis species,
3) whether the liquid is buffered or unbuffered (see Appendix A for the Numerical Technique),
4) temperature of the liquid,
5) temperature of the gas,
6) pressure,
7) average drop surface area diameter,
8) average drop volume diameter,
9) exposure time, and
10) relative error control (see Appendix A for the Numerical Technique).

The output of the program is comprised of three files and two plots. File FOR22.DAT contains a summary of all of the conditions and calculations for the run. File FOR50.DAT contains the concentration of the drop as a function of time and is used to develop the plot of concentration in the liquid versus time. FOR51.DAT contains the gas phase concentration, number of moles of molecular iodine removed per step and the total number of moles removed as a function of time. This file is used to develop a plot of the number of moles removed as a function of

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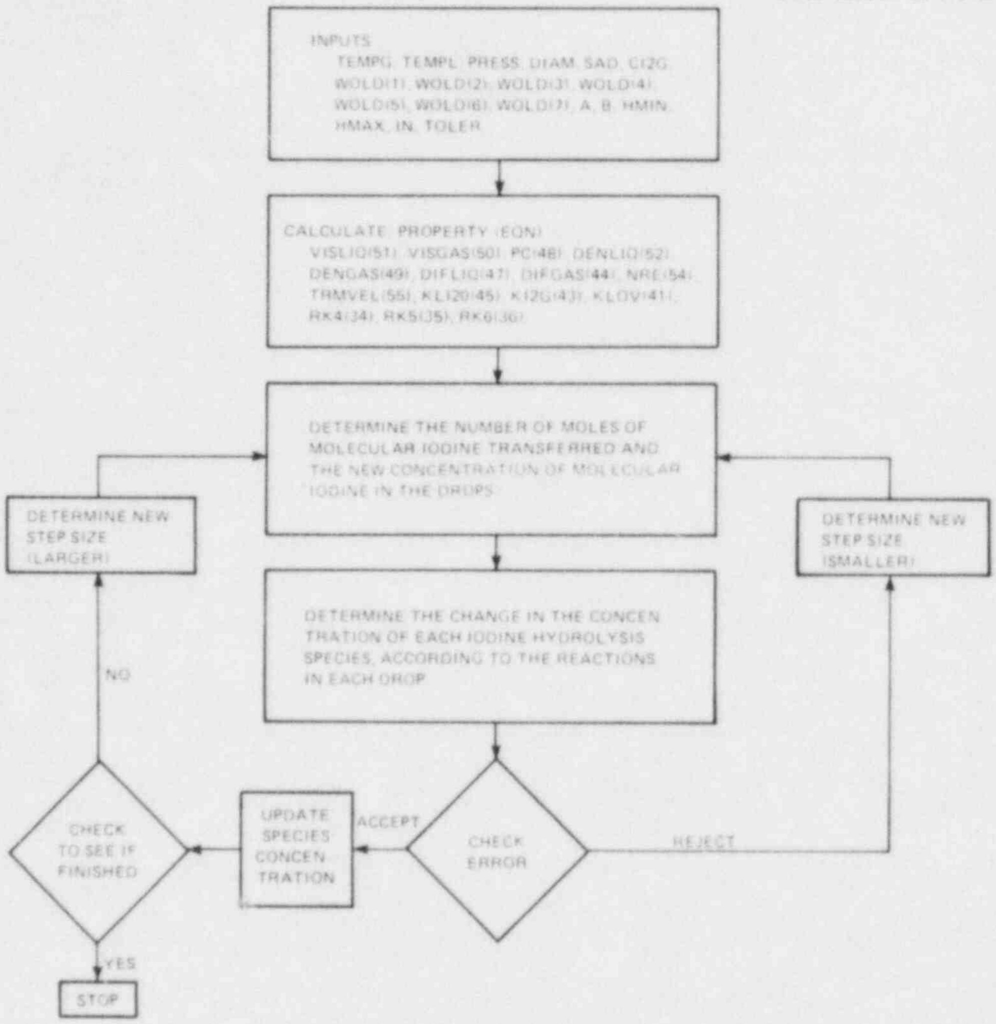

Fig. 14. Drop Model Flowsheet.

time (see Appendix C for sample output files and for the FORTRAN program).

The results of this model are shown in Figures 15 though 26 for cases involving initial concentrations of molecular iodine in the gas phase from 1.0×10^{-5} to 1.0×10^{-10} moles/liter, a drop diameter of 1000 microns, and a temperature of 298 K. Figures 15 through 20 represent the results for cases with a buffered pH of 9.0, and Figures 21 through 26 are for the cases with a buffered pH of 7.0. For each figure part a shows the concentration of the iodine hydrolysis species as a function of time and part b shows the gram-moles of molecular iodine removed as a function of time. If one compares the number of moles of molecular iodine removed per drop for a pH of 7 with the number of moles removed for a buffered pH of 9, it is seen that drops with a pH of 9 remove approximately one and a half times to five times as much iodine from the gas phase as drops with a buffered pH of 7.

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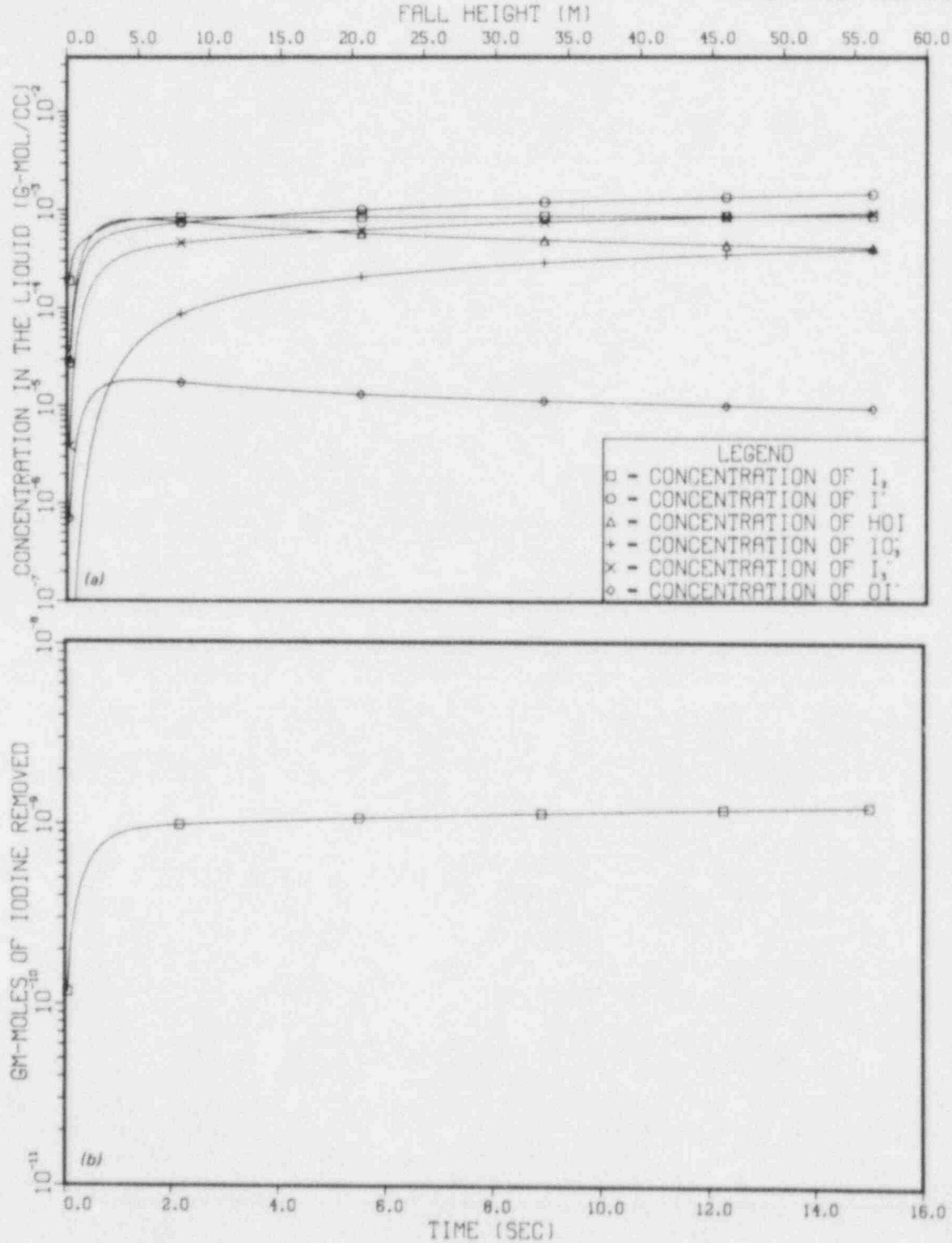

Fig. 15. Results of Drop Model. Initial concentration of molecular iodine in the gas phase of 1.0×10^{-5} moles/liter and a buffered pH of 9.0.
(a) Concentration in the liquid drop as a function of time.
(b) Number of moles of molecular iodine transferred as a function of time.

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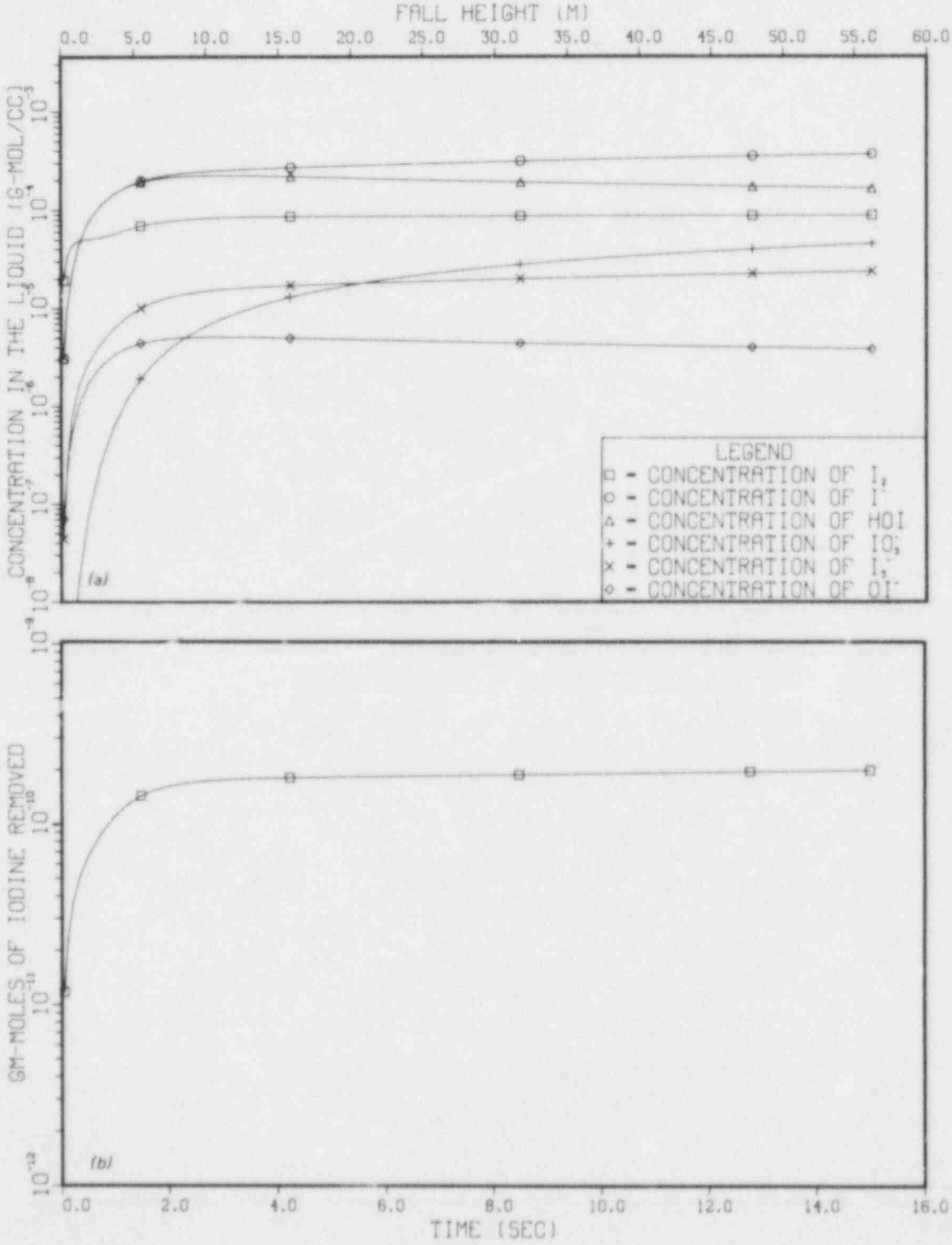

Fig. 16. Results of Drop Model. Initial concentration of molecular iodine in the gas phase of 1.0×10^{-6} moles/liter and a buffered pH of 9.0.

(a) Concentration in the liquid drop as a function of time.

(b) Number of moles of molecular iodine transferred as a function of time.

ORNL-DWG 84-6538 ETD

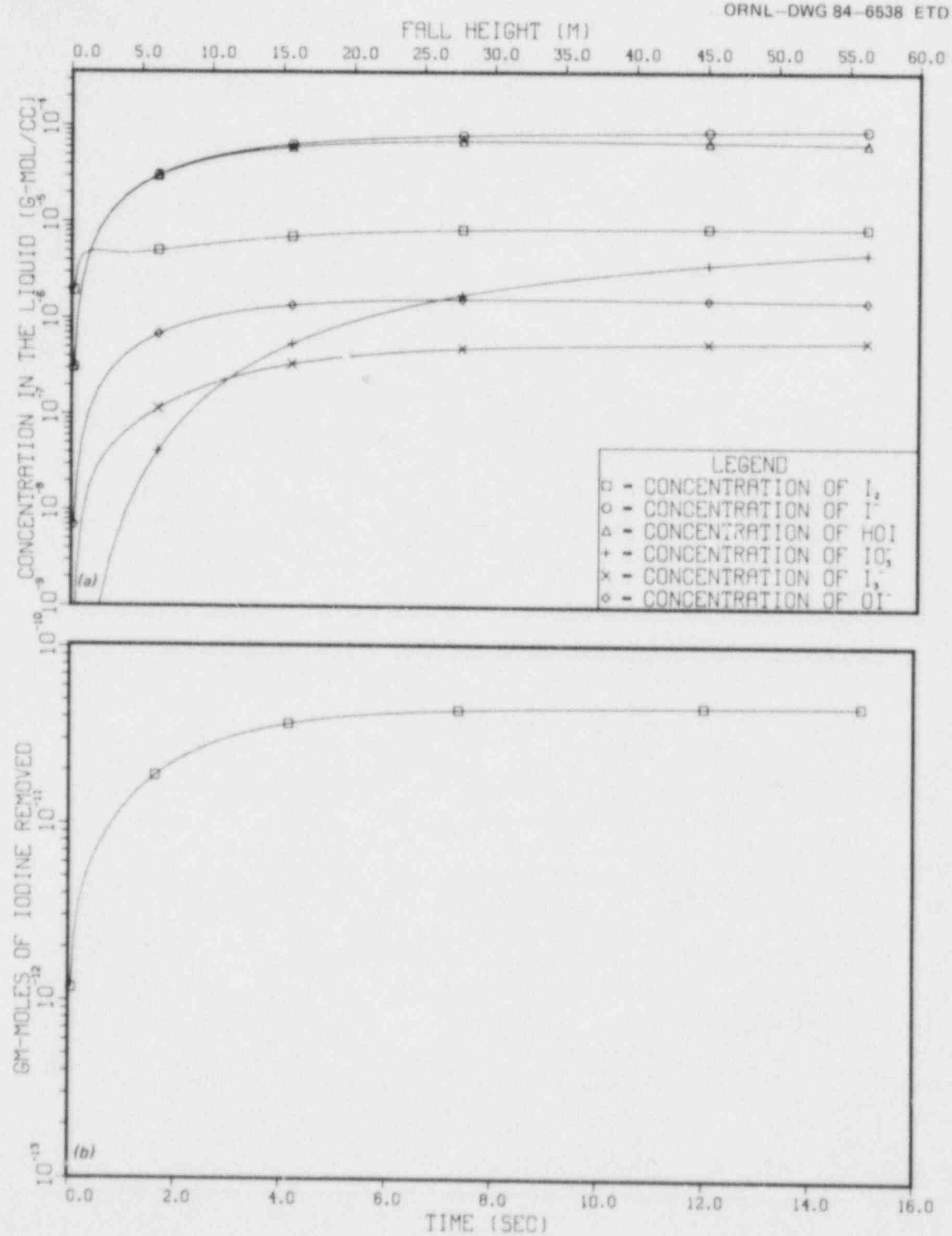

Fig. 17. Results of Drop Model. Initial concentration of molecular iodine in the gas phase of 1.0×10^{-7} moles/liter and a buffered pH of 9.0.

(a) Concentration in the liquid drop as a function of time.

(b) Number of moles of molecular iodine transferred as a function of time.

ORNL-DWG 84-6539 ETD

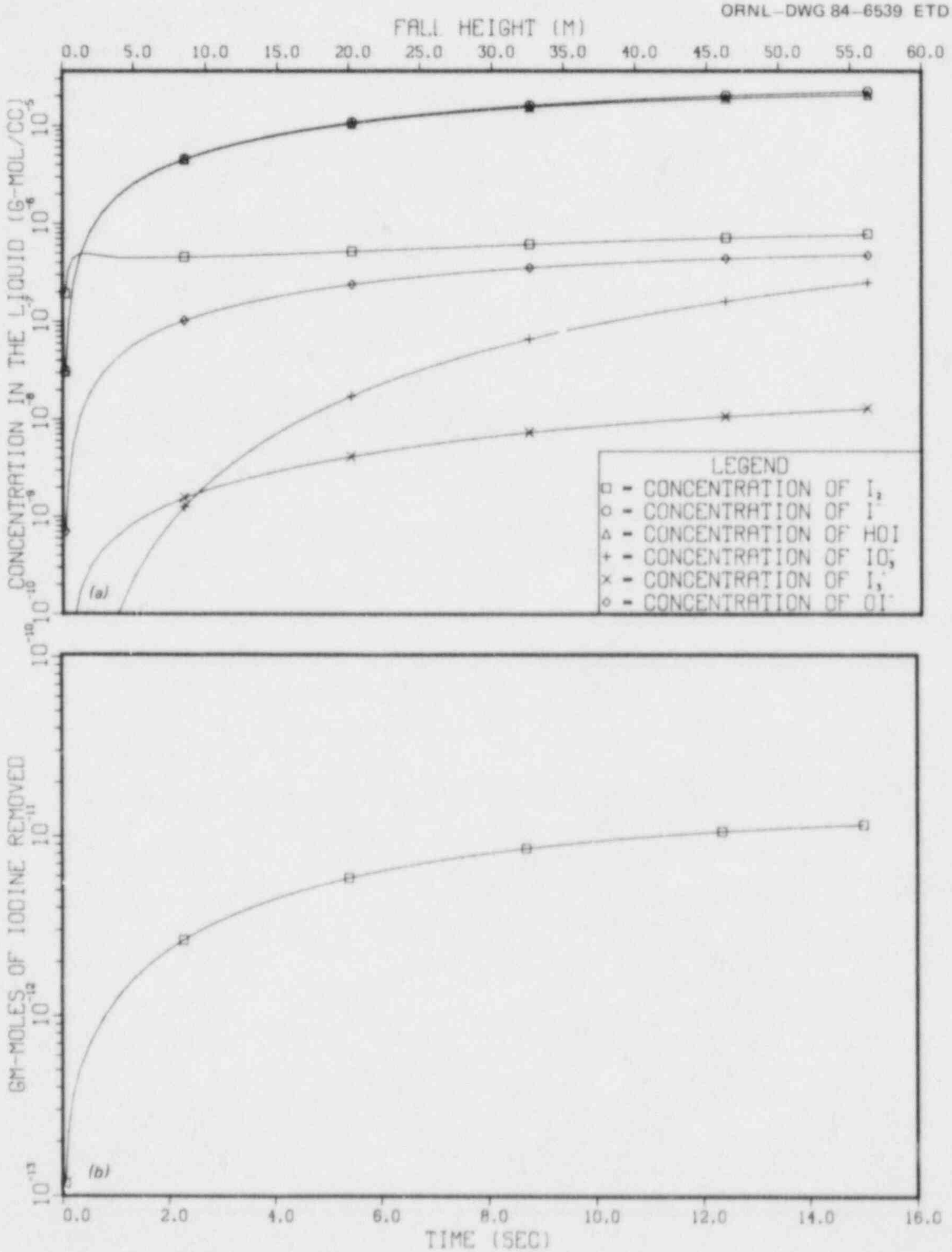

Fig. 18. Results of Drop Model. Initial concentration of molecular iodine in the gas phase of 1.0×10^{-8} moles/liter and a buffered pH of 9.0.

(a) Concentration in the liquid drop as a function of time.

(b) Number of moles of molecular iodine transferred as a function of time.

ORNL-DWG 84-6540 ETD

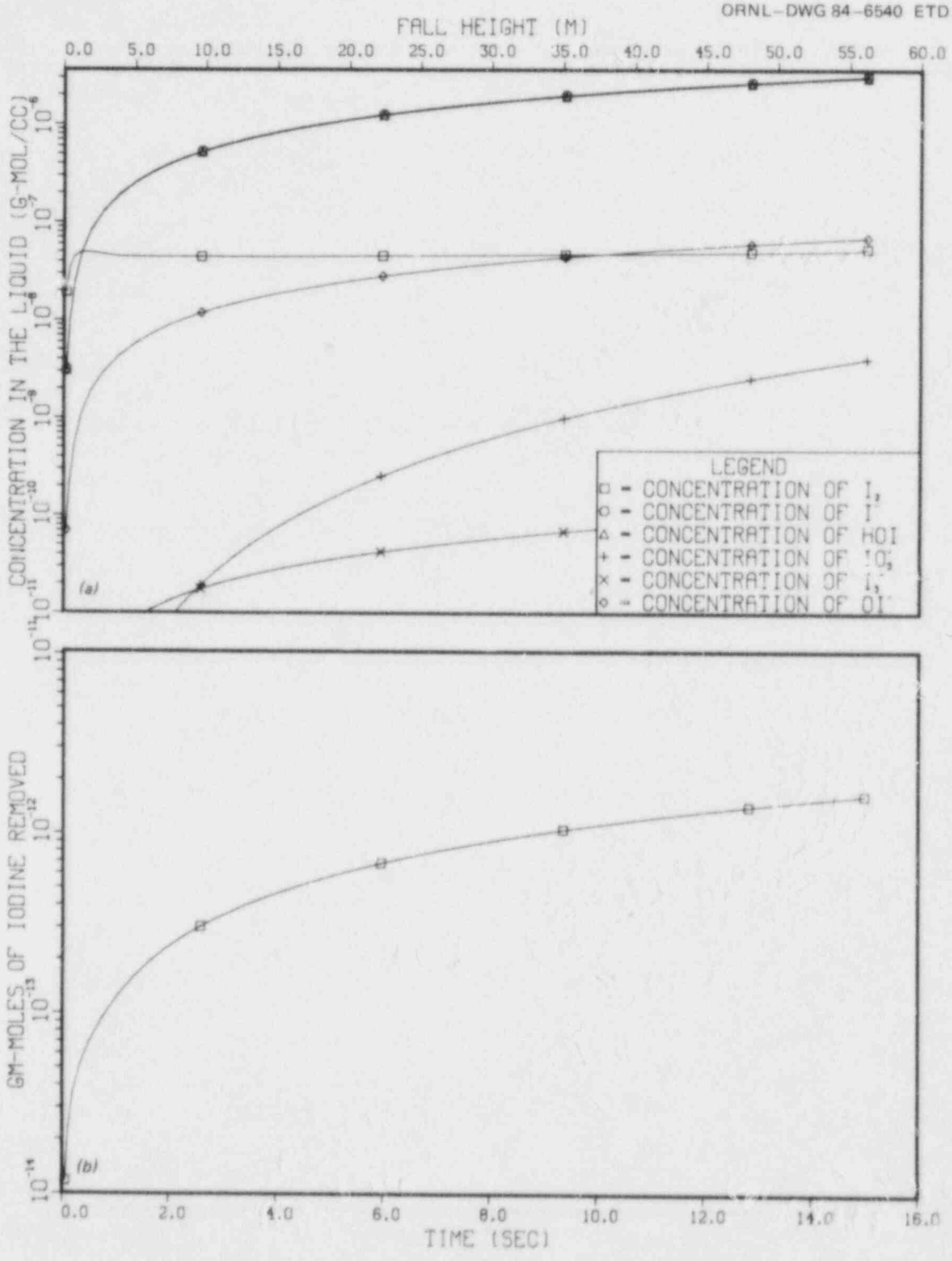

Fig. 19. Results of Drop Model. Initial concentration of molecular iodine in the gas phase of 1.0×10^{-9} moles/liter and a buffered pH of 9.0.

(a) Concentration in the liquid drop as a function of time.

(b) Number of moles of molecular iodine transferred as a function of time.

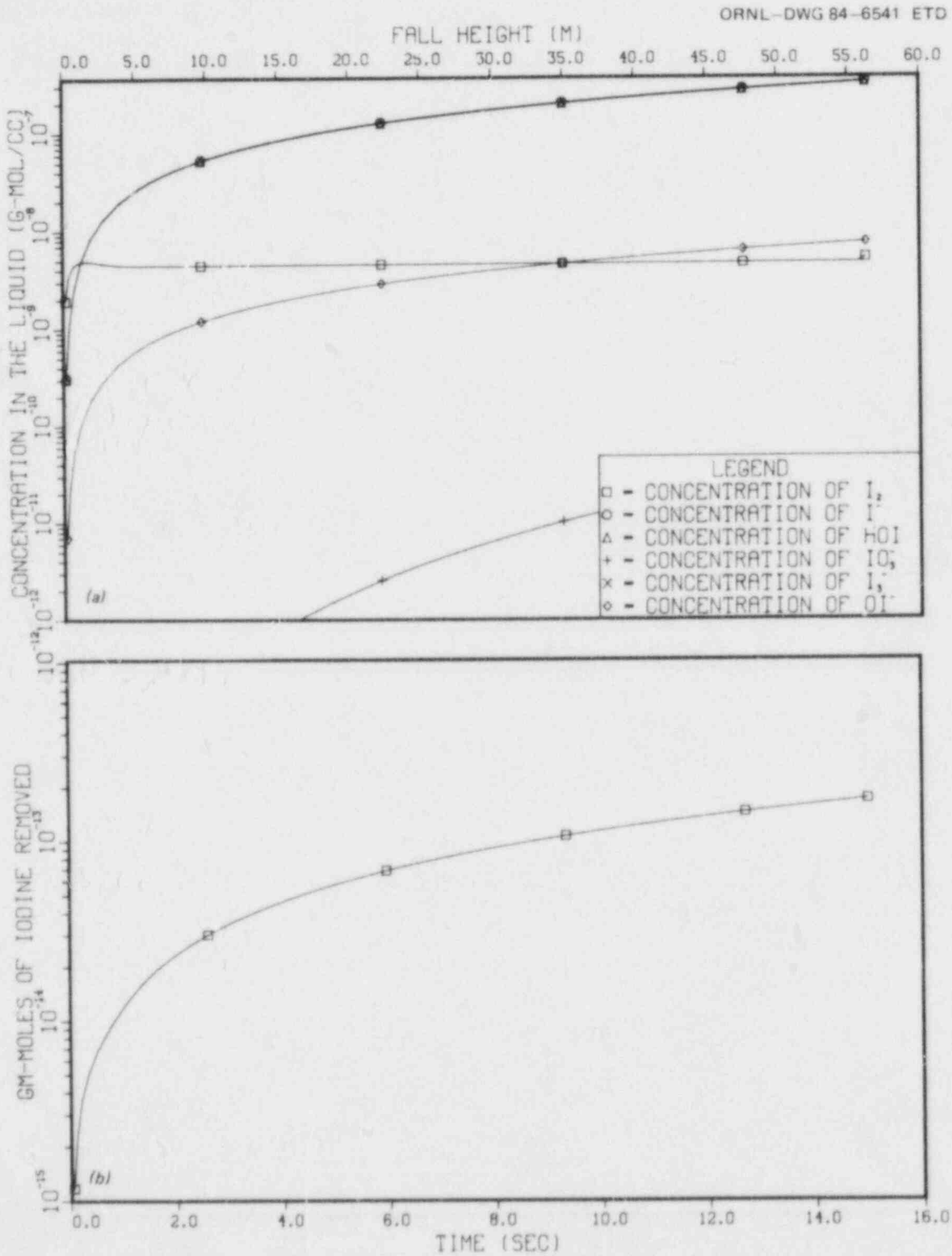

Fig. 20. Results of Drop Model. Initial concentration of molecular iodine in the gas phase of 1.0×10^{-10} moles/liter and a buffered pH of 9.0.

(a) Concentration in the liquid drop as a function of time.

(b) Number of moles of molecular iodine transferred as a function of time.

ORNL-DWG 84-6543 ETD

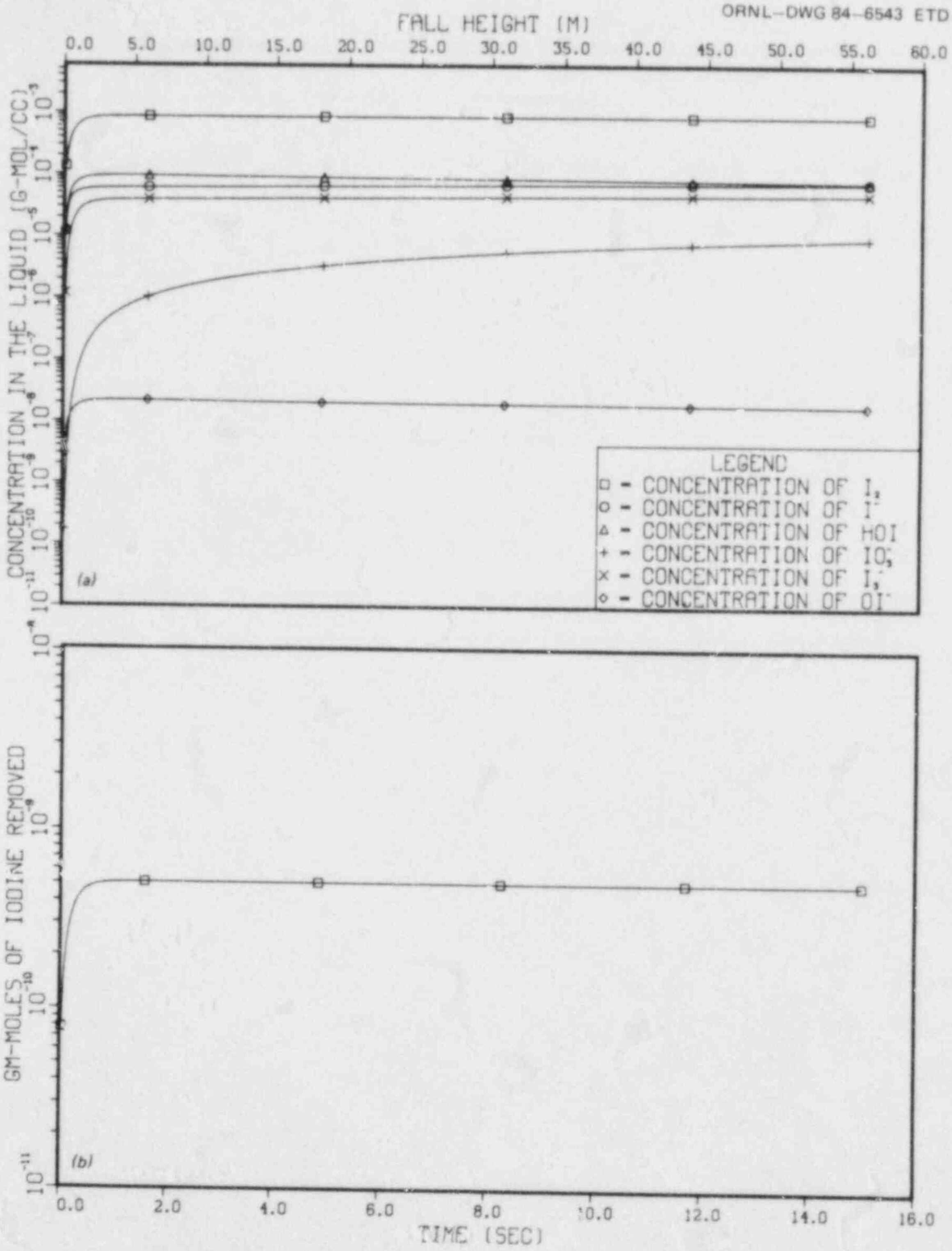

Fig. 21. Results of Drop Model. Initial concentration of molecular iodine in the gas phase of 1.0×10^{-5} moles/liter and a buffered pH of 7.0.

(a) Concentration in the liquid drop as a function of time.

(b) Number of moles of molecular iodine transferred as a function of time.

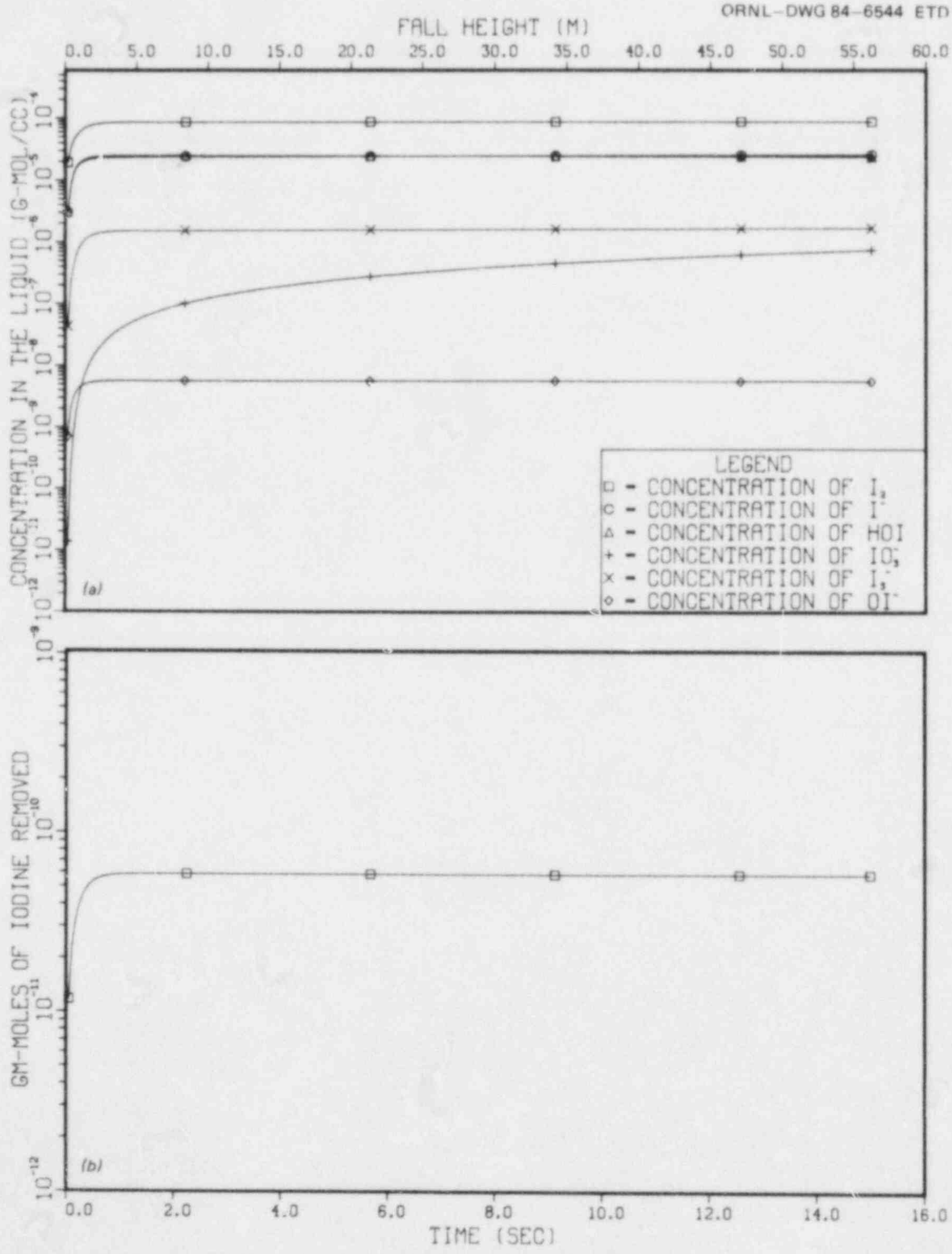

Fig. 22. Results of Drop Model. Initial concentration of molecular iodine in the gas phase of 1.0×10^{-6} moles/liter and a buffered pH of 7.0.

(a) Concentration in the liquid drop as a function of time.

(b) Number of moles of molecular iodine transferred as a function of time.

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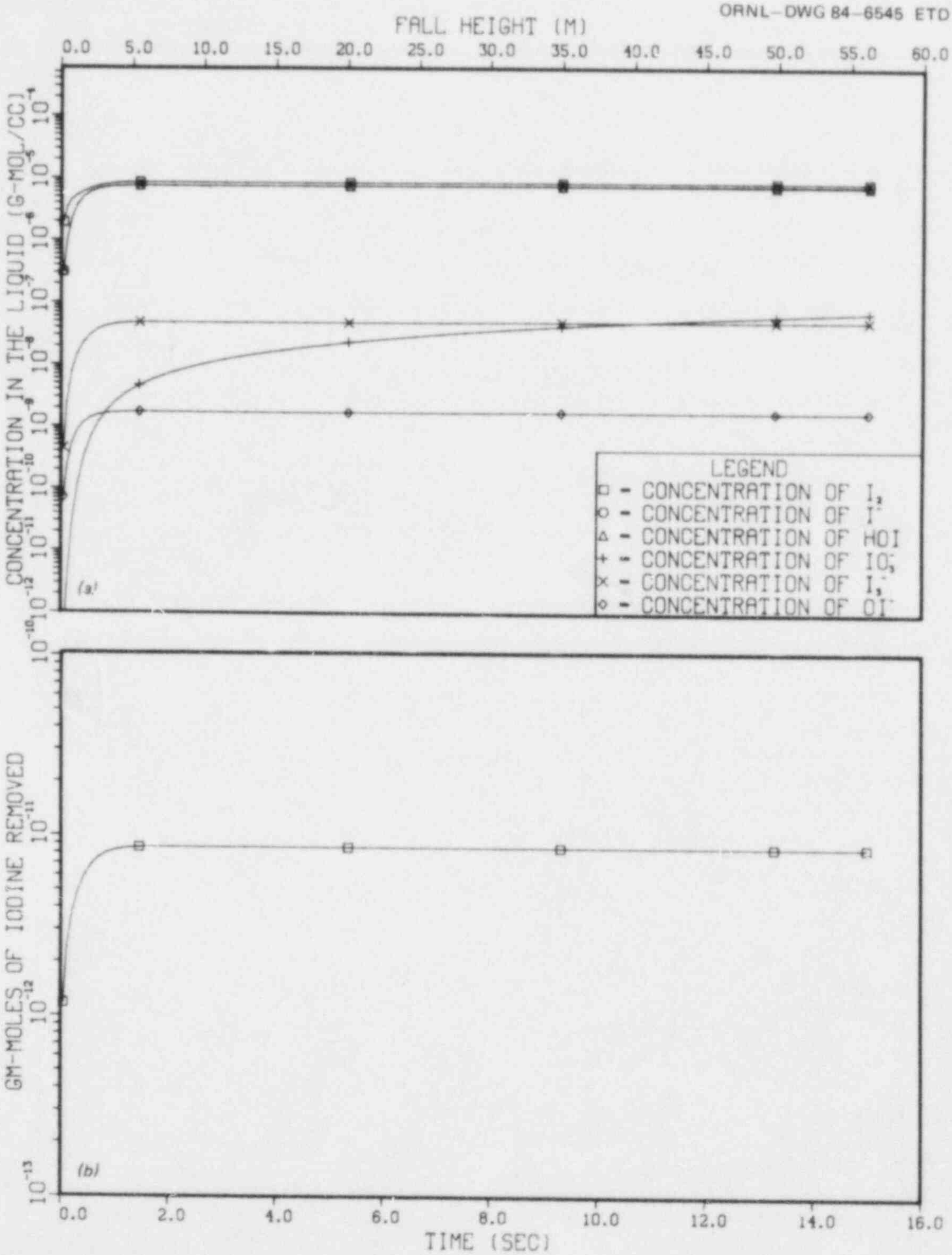

Fig. 23. Results of Drop Model. Initial concentration of molecular iodine in the gas phase of 1.0×10^{-7} moles/liter and a buffered pH of 7.0.

(a) Concentration in the liquid drop as a function of time.

(b) Number of moles of molecular iodine transferred as a function of time.

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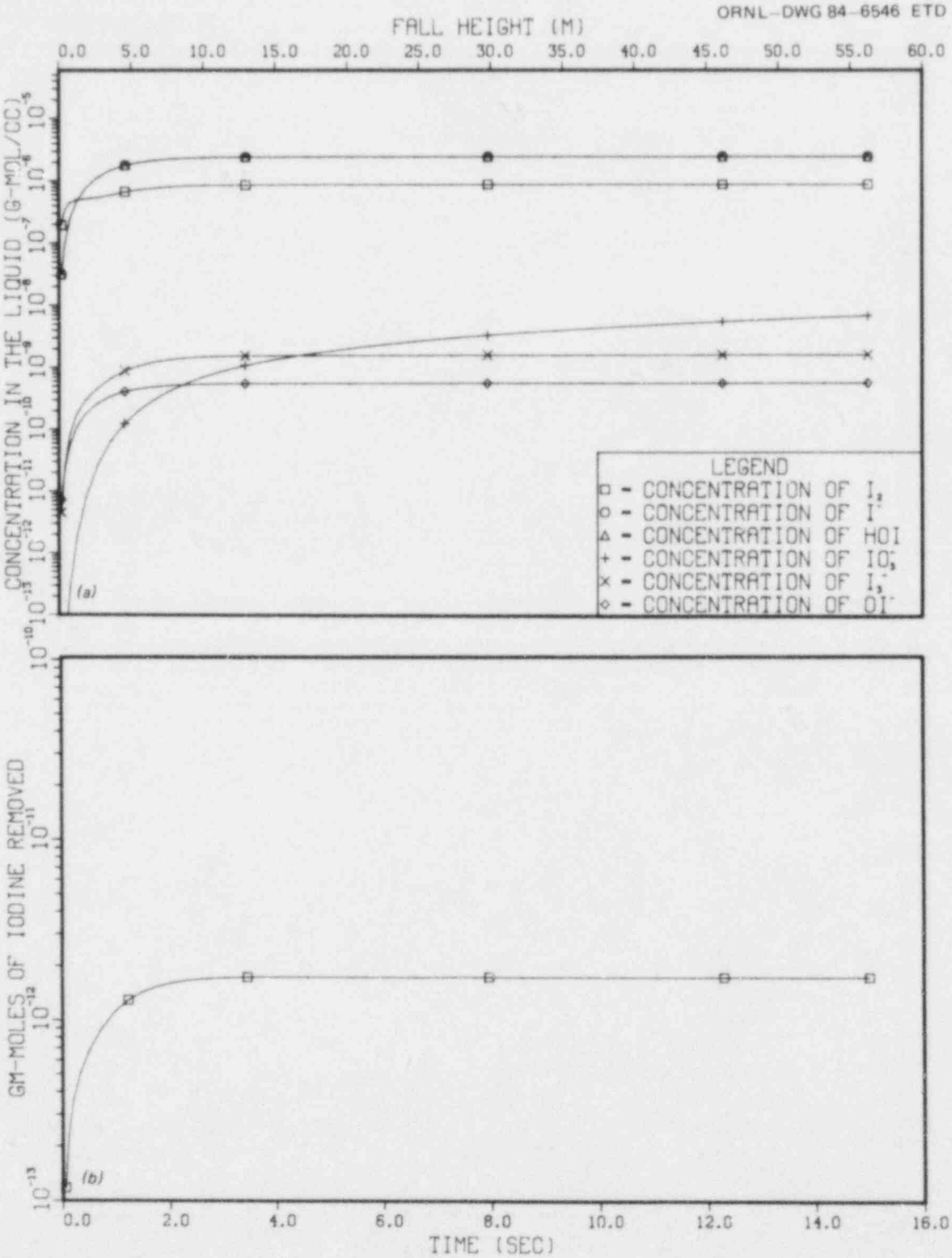

Fig. 24. Results of Drop Model. Initial concentration of molecular iodine in the gas phase of 1.0×10^{-8} moles/liter and a buffered pH of 7.0.

(a) Concentration in the liquid drop as a function of time.

(b) Number of moles of molecular iodine transferred as a function of time.

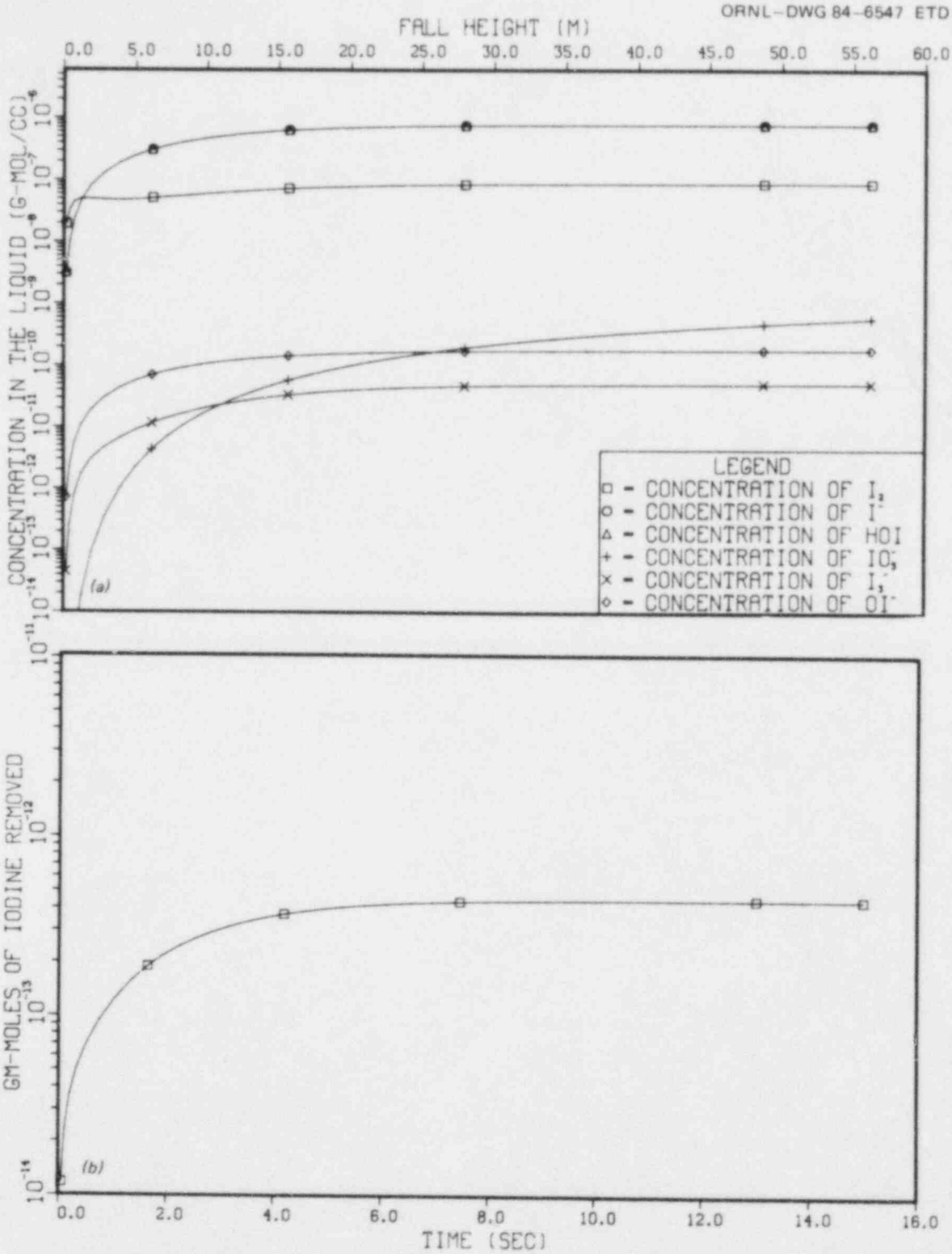

Fig. 25. Results of Drop Model. Initial concentration of molecular iodine in the gas phase of 1.0×10^{-9} moles/liter and a buffered pH of 7.0.

(a) Concentration in the liquid drop as a function of time.

(b) Number of moles of molecular iodine transferred as a function of time.

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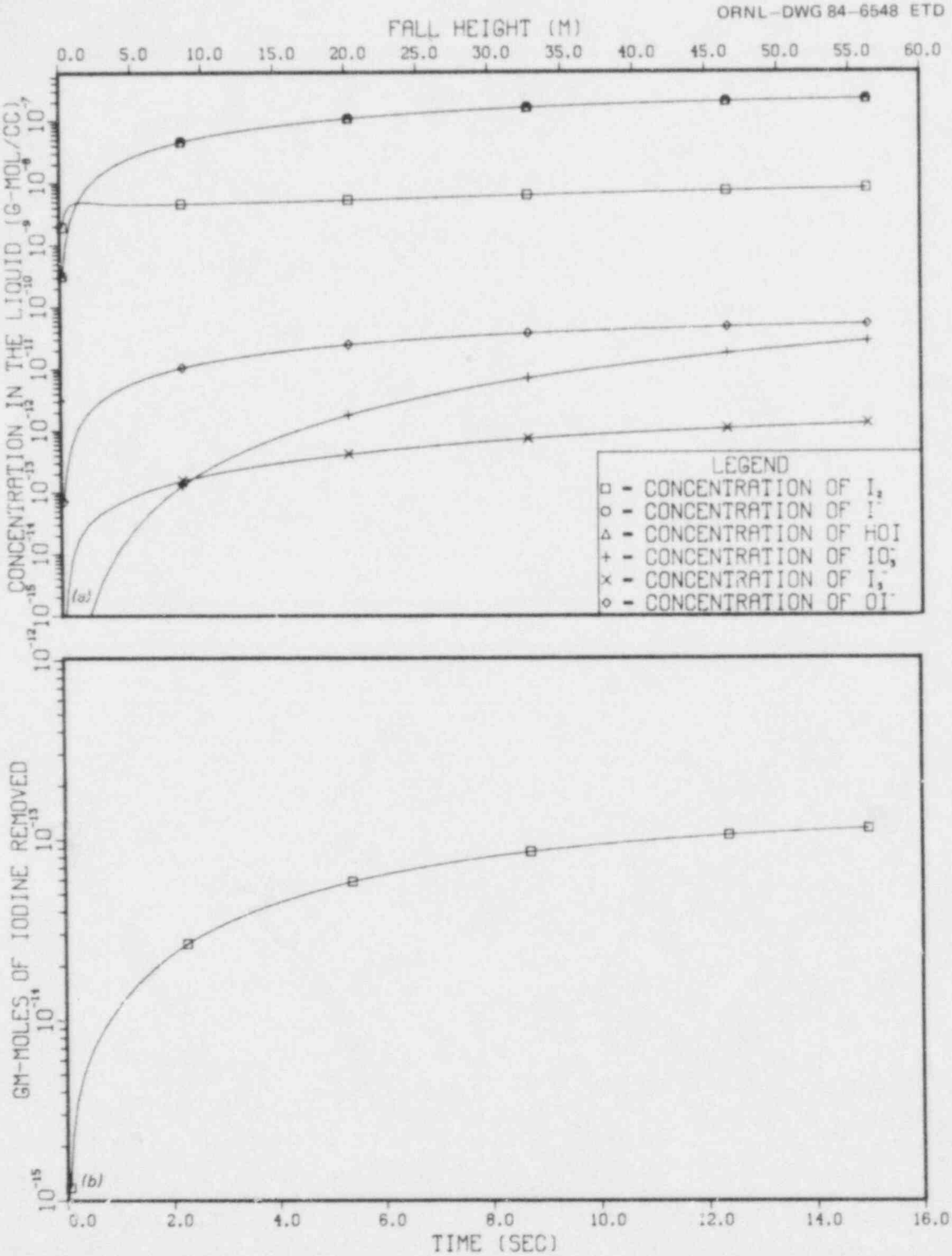

Fig. 26. Results of Drop Model. Initial concentration of molecular iodine in the gas phase of 1.0×10^{-10} moles/liter and a buffered pH of 7.0.

(a) Concentration in the liquid drop as a function of time.

(b) Number of moles of molecular iodine transferred as a function of time.

5. SPRAY MODEL

The spray model is an expansion of the single droplet model into a spray system. The drop model is expanded to be applicable to a system of many drops suspended in a gas during the period of the drop fall time. The assumptions for the spray model are:

1) each drop has a completely mixed bulk liquid,
2) resistance to mass transfer exists in both the gas phase and the liquid phase,
3) molecular iodine (I_2) is the only species that transfers (has volatility) in or out of the drop,
4) reactions occur in the bulk of the liquid,
5) each drop falls at its terminal velocity,
6) every drop falls the same height,
7) each drop has a constant surface area and constant volume at all times,
8) there are no interactions between drops,
9) for the lifetime of a drop, the physical characteristics of the gas phase remains constant but the gas phase concentration can change slowly in a stepwise fashion over several drop lifetimes,
10) there is no transfer of heat or water between the drop and the gas phase (see Chapter 4, DROP MODEL), and
11) the containment height is the same as the drop fall height.

These assumptions are the same as for the drop model except for assumptions 6, 8, and 11. Both assumptions 6 and 8 deal with the relationship each drop has with the other drops and therefore would not be present in a single drop model. Assumption 11 is needed to calculate the containment volume, CVOL, by:

$$CVOL = \pi \; CDIAM^2 \; HEIGHT/4.0 \; , \tag{56}$$

where

CDIAM = containment diameter, and
HEIGHT = drop fall height.

Since all drops are assumed to fall at the same velocity and fall the same height, their exposure time will be the same. The total duration of the spray can be broken into N segments, where N is determined by:

$$N = \frac{\text{total spray time}}{\text{drop exposure time}} \; . \tag{57}$$

The spray model determines the total volume and surface area of all of the drops suspended in the gas at any instant. The surface-to-volume ratio of one large drop having this volume and surface area will not be

the same as the surface-to-volume ratio for the small drops, and the large drop would have to be significantly non-spherical. Nevertheless, the total volume and surface area is used to simulate one large non-spherical drop in which the drop model is applied to this large drop for N times. The algorithm used is (see Figure 27 for spray model flow-sheet):

1) determine all physical properties for the gas and liquid phases,
2) determine the number of loops required, (N),
3) determine the total surface area and total volume for all of the drops in containment,
4) execute the drop model for the large drop with surface area and volume equilvalent to these quantities for the actual system:
   a) determine the number of moles of molecular iodine that are transferred to the large drop from the gas phase,
   b) calculate the concentration of molecular iodine in the large liquid drop,
   c) determine the concentration of all species in the large liquid drop due to the iodine hydrolysis reactions,
5) calculate the new gas phase concentration, and
6) loop to step 4 until N loops have been completed.

A FORTRAN program that implements this algorithm is listed in Appendix E. Input parameters for the spray model are:

1) initial gas phase concentration of molecular iodine,
2) initial liquid phase concentration of all iodine hydrolysis species,
3) whether the liquid phase is buffered or unbuffered (see Appendix A, Numerical Technique)
4) temperature of both gas and liquid phases,
5) pressure,
6) average drop surface area diameter,
7) average drop volume diameter,
8) spray time,
9) spray flow rate,
10) drop fall height,
11) containment diameter, and
12) relative error control (see Appendix A, Numerical Technique).

Output from the program comprises four files and four plots. File FOR22.DAT contains a summary of all of the conditions and calculations of the run. File FOR50.DAT contains the concentration of the drops when they have fallen a distance equal to their input fall height and is used to create a plot of the concentration in the liquid drops versus time. File FOR51.DAT contains the gas phase concentration of molecular iodine, number of moles removed for each individual group of drops and the total number of moles removed versus time. FOR51.DAT is used to create a plot of concentration of molecular iodine removed versus time, and a plot of the number of moles of iodine versus time. File FOR52.DAT contains the concentration of the sprayed solution collected in the sump, and is used to create a plot of the concentration of iodine in the sump versus time.

ORNL-DWG 84-6610

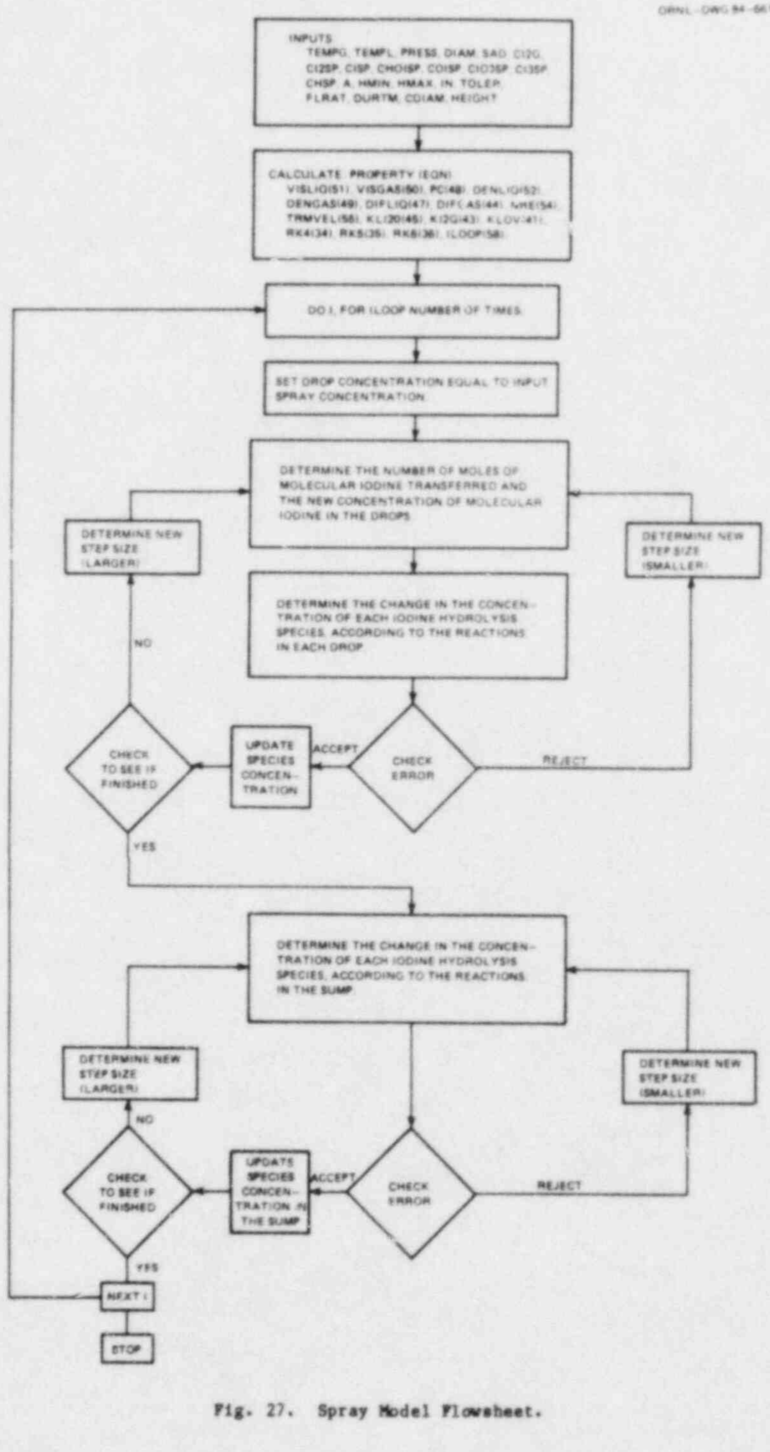

Fig. 27. Spray Model Flowsheet.

A series of computer runs was performed for initial concentrations of molecular iodine in the gas phase from 1×10^{-5} through 1.0×10^{-10} moles/liter for 10 minute sprays times. Results for the cases with a buffered pH of 9 are shown in Figures 28 through 33 and results for the cases with a buffered pH of 7 are shown in Figures 34 through 39. The common inputs to the computer program for the cases whose results are shown in these figures are:

1) the initial liquid phase species concentrations are all zero except for the hydrogen ion concentration,
2) all of the spray solutions are buffered at pH 9 or pH 7,
3) the temperature of the gas is 298K and the temperature of the liquid is 298K,
4) the pressure is 1 atmosphere,
5) the drop surface area diameter is 0.1 centimeters,
6) the drop volume diameter is 0.1 centimeter,
7) the spray time is 10 minutes,
8) the spray flow rate is 37 liters/minute,
9) the drop fall height is 15.4 meters, and
10) the containment diameter is 3.3 meters.

These inputs were arbitrarily chosen, but are within the range of conditions that are likely to be encountered in potential reactor accident systems.

For these input parameters, Figures 28 to 39 show the results of these series of runs. Part a of each Figure shows the concentration of molecular iodine in the gas phase as a function of time. For the conditions of these tests, the gas phase concentration does not change very much. (This result is only valid for the conditions of these runs.) Part b of each Figure shows the number of gram-moles of molecular iodine removed versus time. These plots show a first order removal (a constant amount of molecular iodine is being removed between each time step). This is because the gas phase concentration of molecular iodine is remaining relatively constant. (Again this is only true for these conditions.) Part c of each Figure shows the concentration in the drops when they have fallen a distance equal to their fall height. These plots show that the concentration in the drops is not changing very much which is again because the gas phase concentration is not changing. Finally part d shows the concentration of iodine in the sprayed solution that is collecting in the sump at the bottom of the containment. The concentration of molecular iodine in the sump decreases slowly with time because the solution is becoming slightly more diluted from the slightly lower concentration of molecular iodine in the drops and also because of the iodine hydrolysis reactions that are occurring in the sump.

A typical run on a Digital Equipment Corporation PDP-10 takes approximately 6 seconds of central processing unit (CPU) time for every minute of simulation. The CPU time depends upon the concentration of molecular iodine, the pH of the solution, whether it is buffered or unbuffered, and the error tolerance. For these simulations of 10 minutes of problem time, each run takes approximately 1 minute of CPU time.

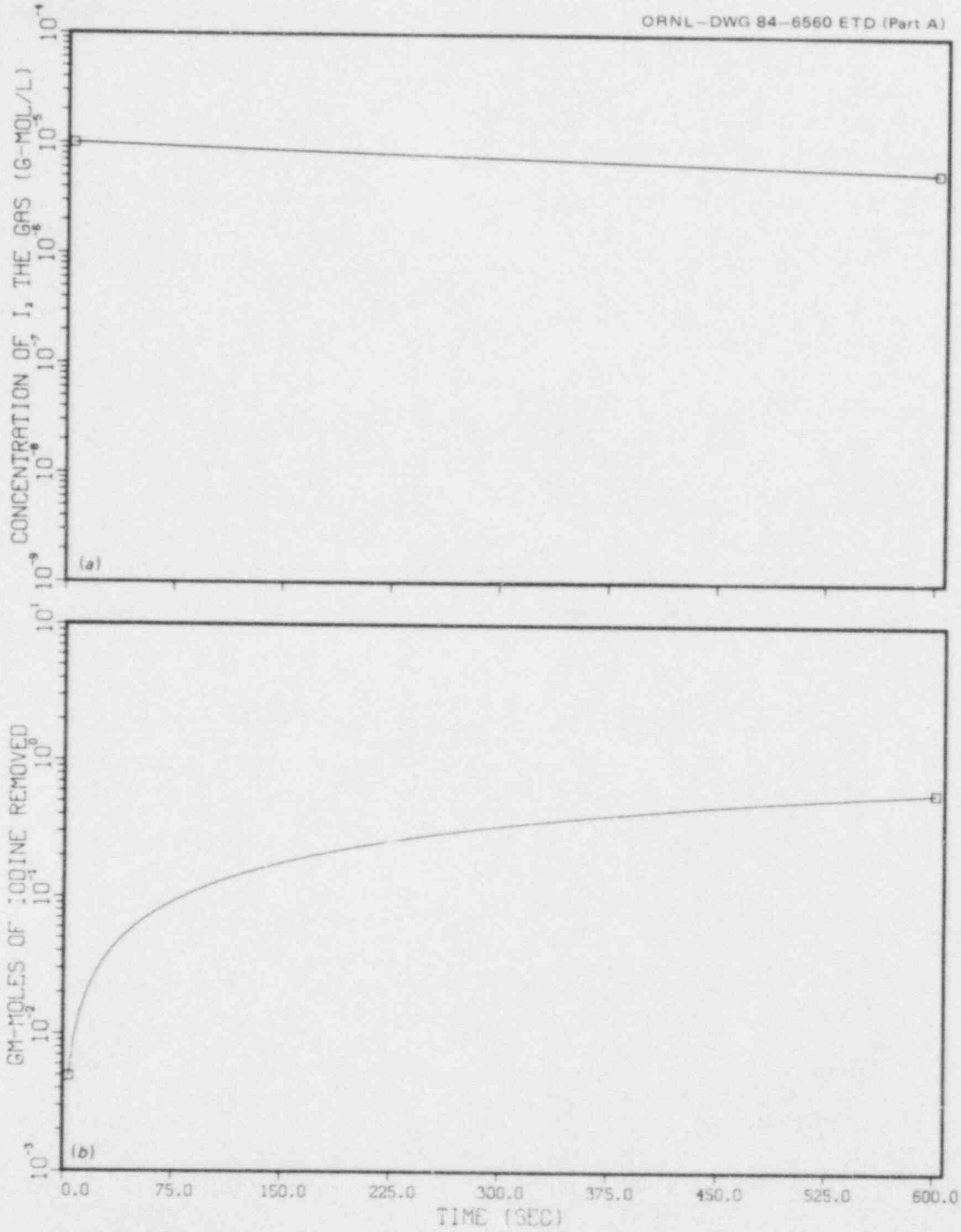

Fig. 28. Results of Spray Model. Initial concentration of molecular iodine in the gas phase of 1×10^{-5} moles/liter and a buffered pH of 9.0 in the liquid phase.

(a) Concentration of molecular iodine in the gas phase as a function of time.

(b) Number of moles of molecular iodine transferred as a function of time.

(c) Concentration of iodine species in the liquid drops as a function of time.

(d) Concentration of iodine species in the sump as a function of time.

ORNL-DWG 84-6560 ETD (Part B)

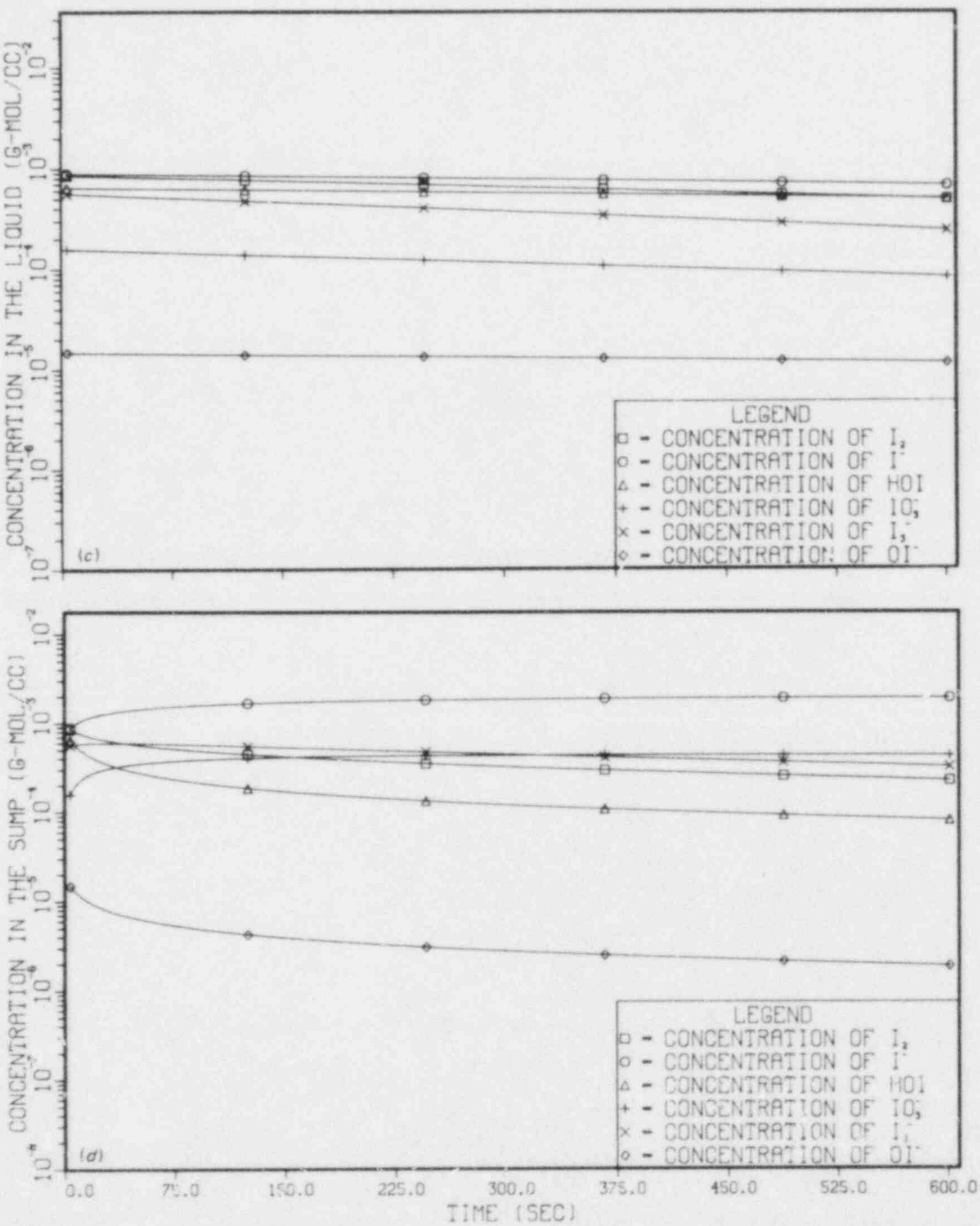

Fig. 28. (continued).

ORNL–DWG 84–6561 ETD (Part A)

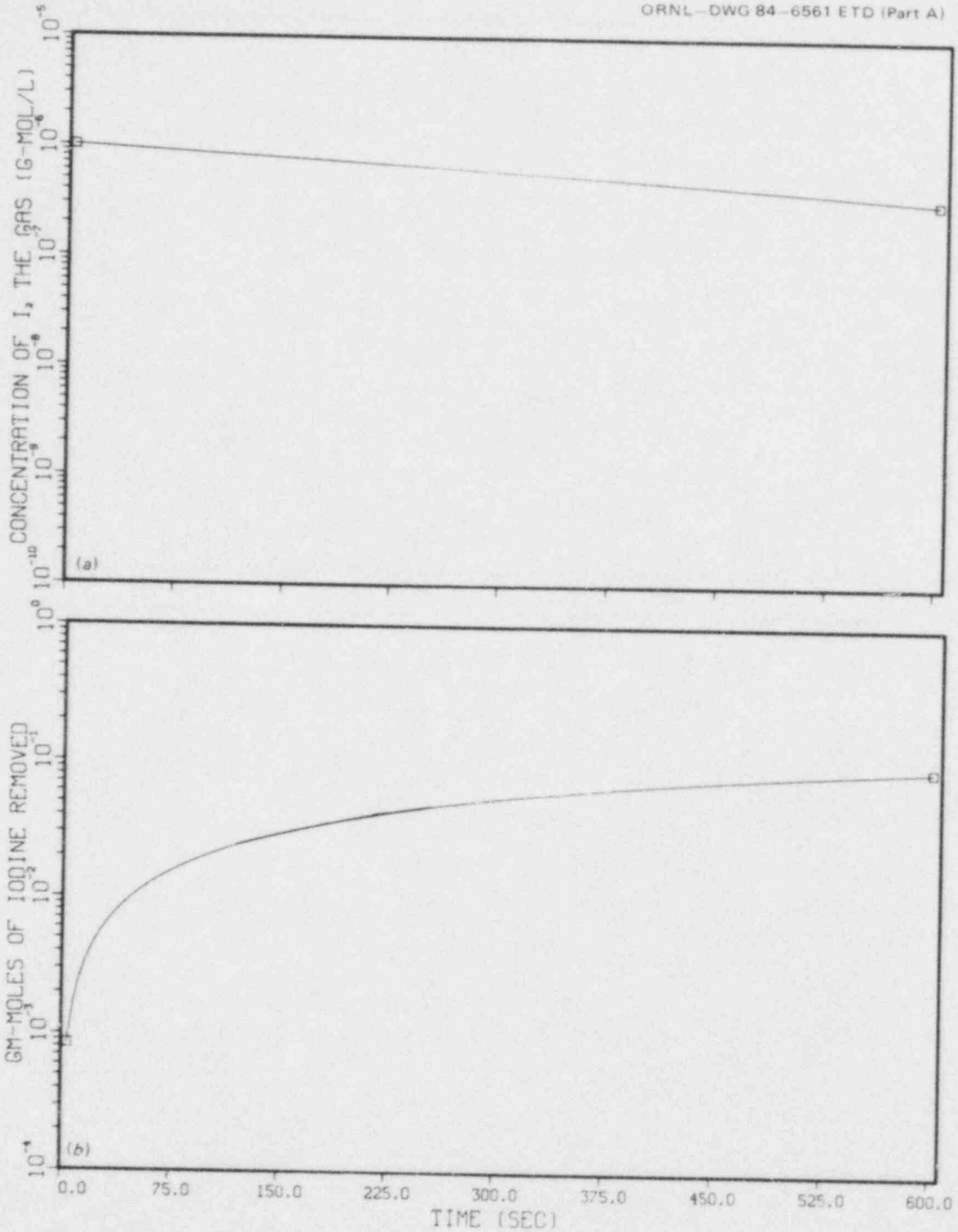

Fig. 29. Results of Spray Model. Initial concentration of molecular iodine in the gas phase of 1×10^{-6} moles/liter and a buffered pH of 9.0 in the liquid phase.

(a) Concentration of molecular iodine in the gas phase as a function of time.

(b) Number of moles of molecular iodine transferred as a function of time.

(c) Concentration of iodine species in the liquid drops as a function of time.

(d) Concentration of iodine species in the sump as a function of time.

ORNL-DWG 84-6561 ETD (Part B)

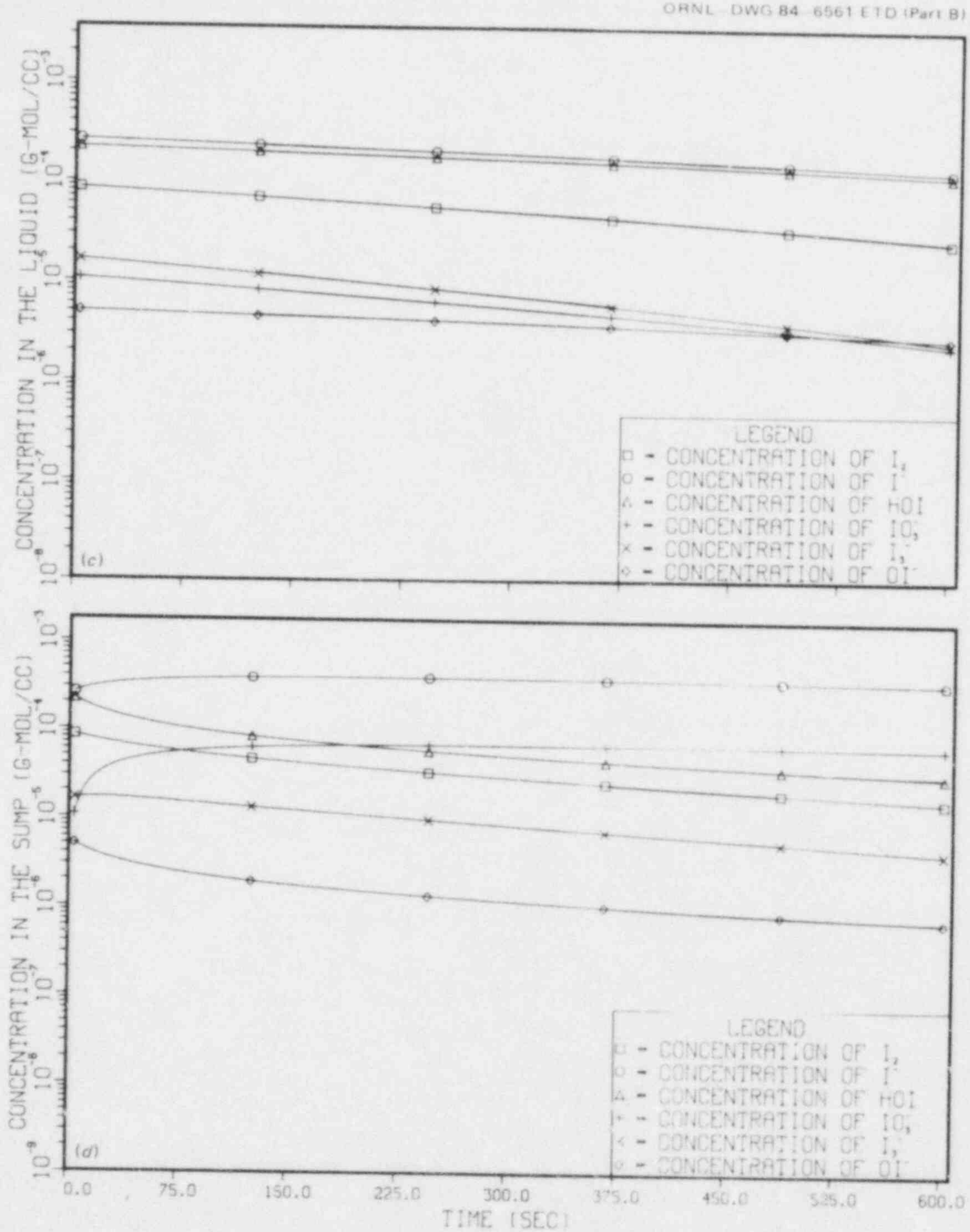

Fig. 29. (continued).

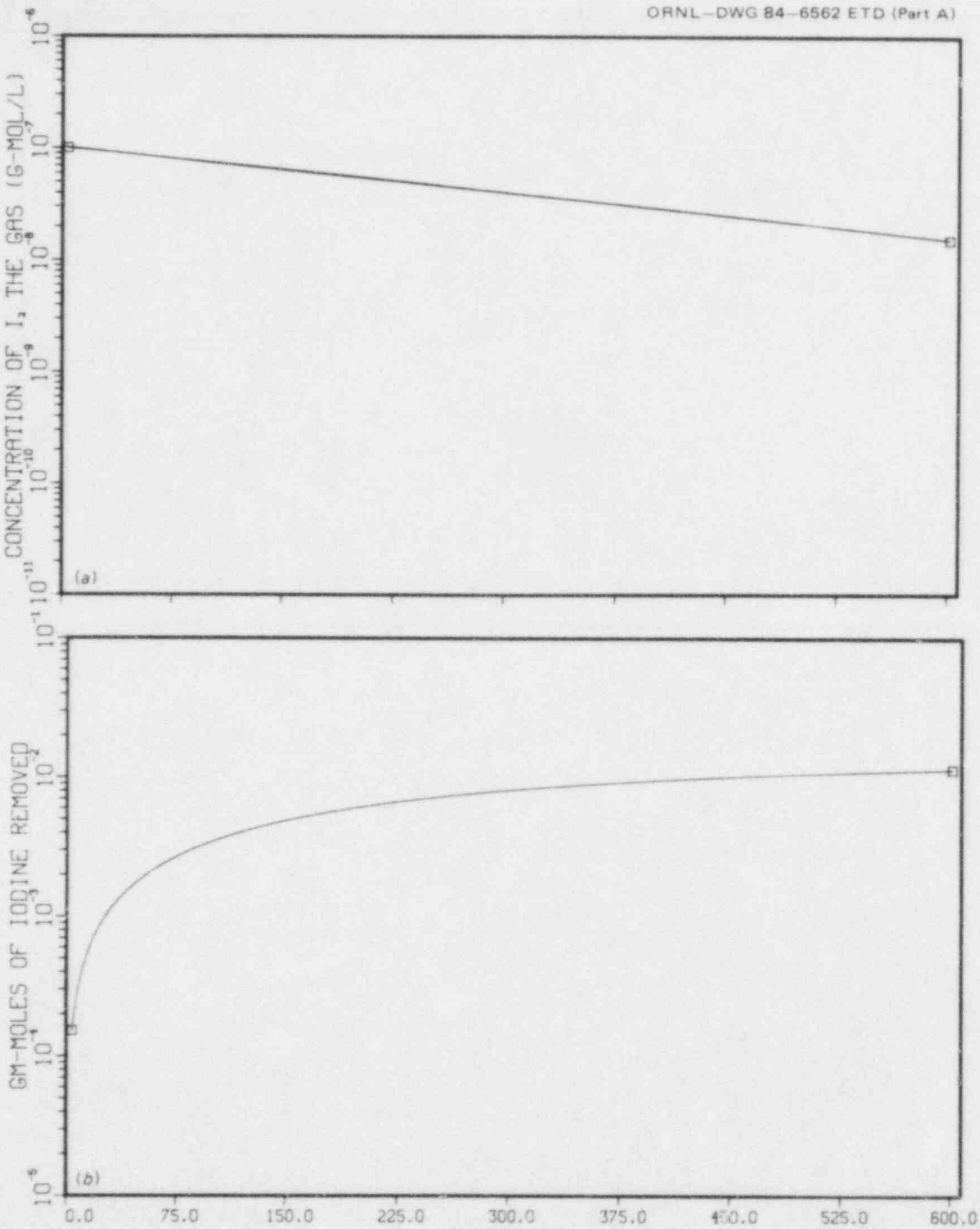

Fig. 30. Results of Spray Model. Initial concentration of molecular iodine in the gas phase of 1×10^{-7} moles/liter and a buffered pH of 9.0 in the liquid phase.

(a) Concentration of molecular iodine in the gas phase as a function of time.

(b) Number of moles of molecular iodine transferred as a function of time.

(c) Concentration of iodine species in the liquid drops as a function of time.

(d) Concentration of iodine species in the sump as a function of time.

ORNL—DWG 84—6562 ETD (Part B)

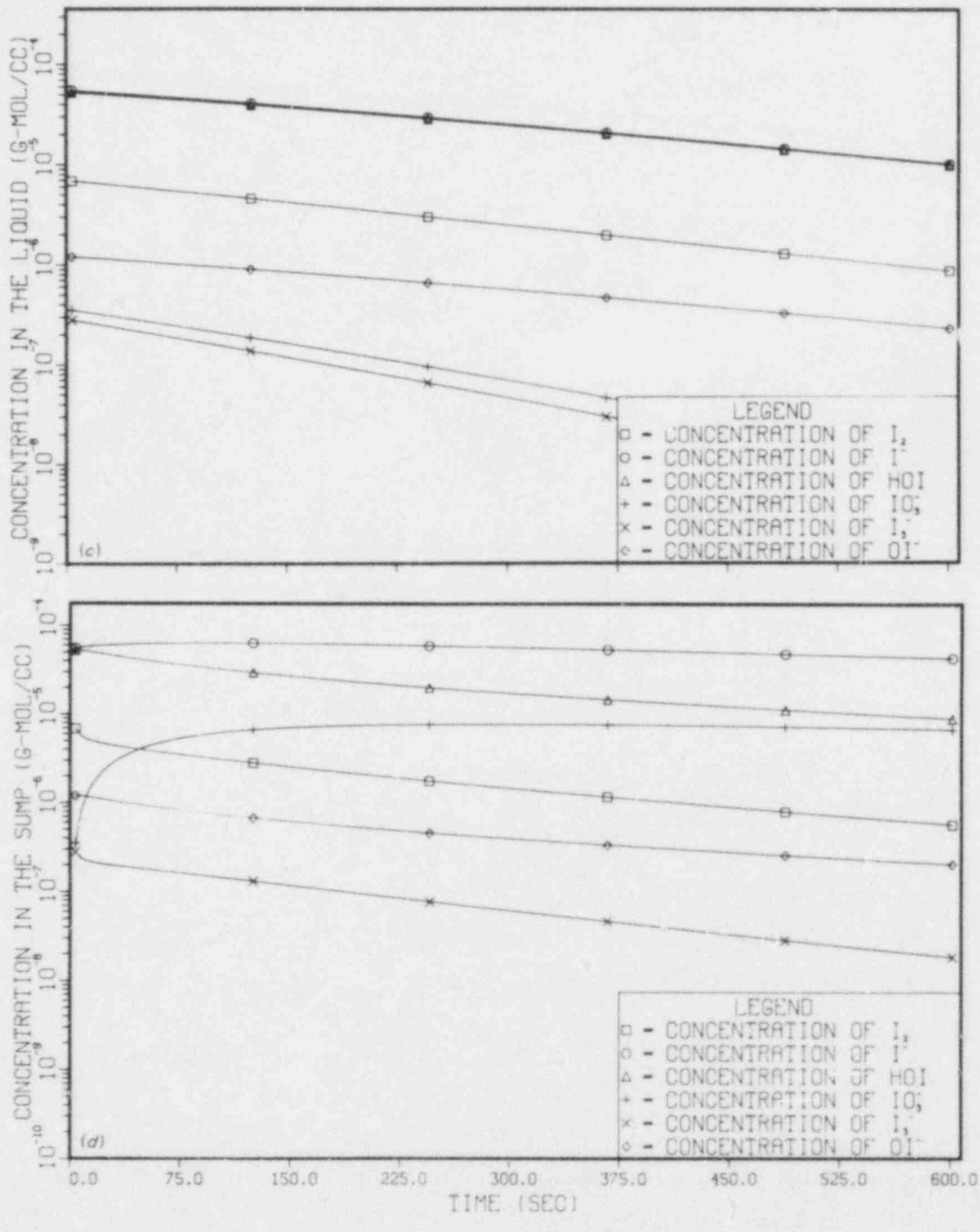

Fig. 30. (continued).

ORNL–DWG 84–6563 ETD (Part A)

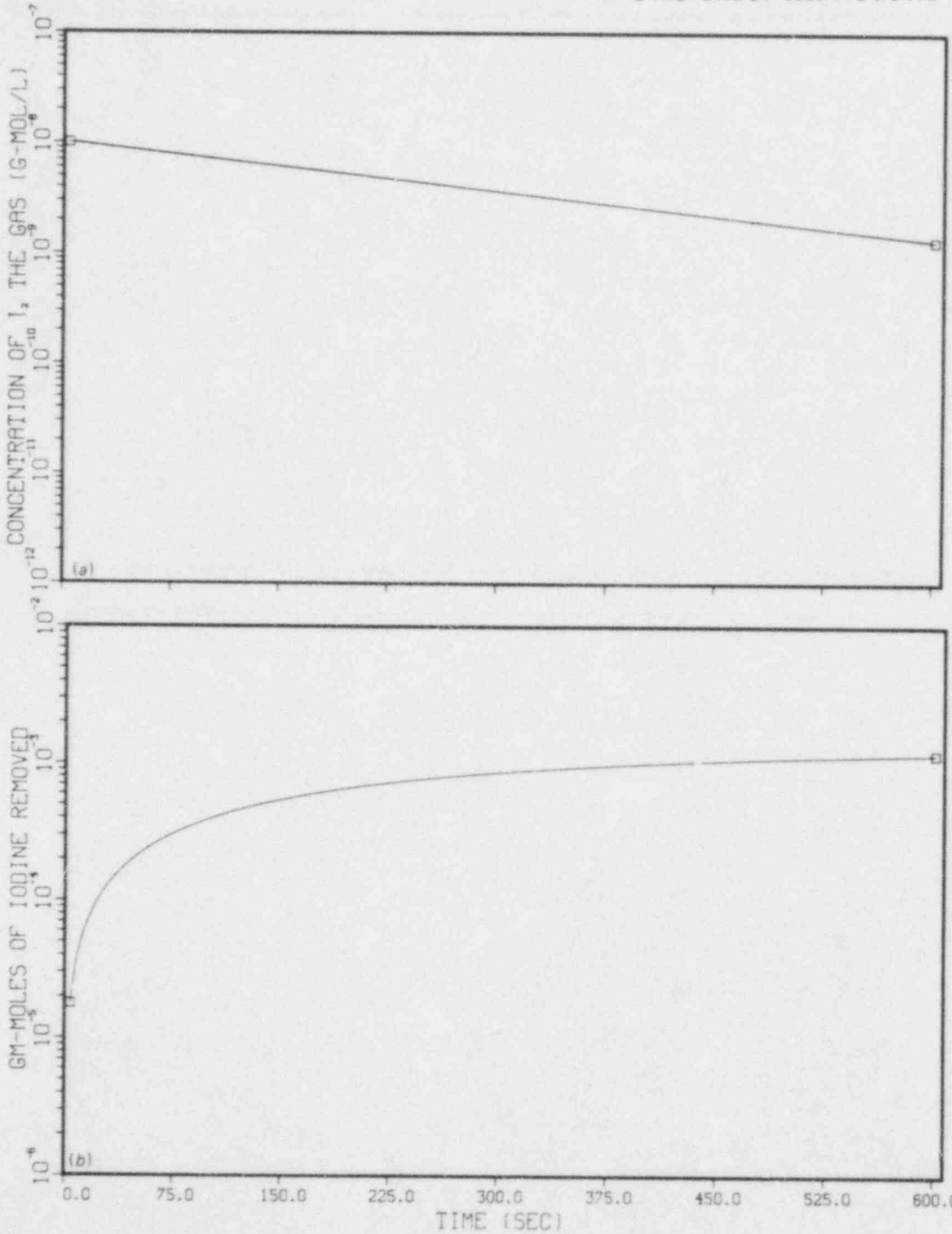

Fig. 31. Results of Spray Model. Initial concentration of molecular iodine in the gas phase of 1×10^{-8} moles/liter and a buffered pH of 9.0 in the liquid phase.

(a) Concentration of molecular iodine in the gas phase as a function of time.

(b) Number of moles of molecular iodine transferred as a function of time.

(c) Concentration of iodine species in the liquid drops as a function of time.

(d) Concentration of iodine species in the sump as a function of time.

ORNL-DWG 84-6563 ETD (Part B)

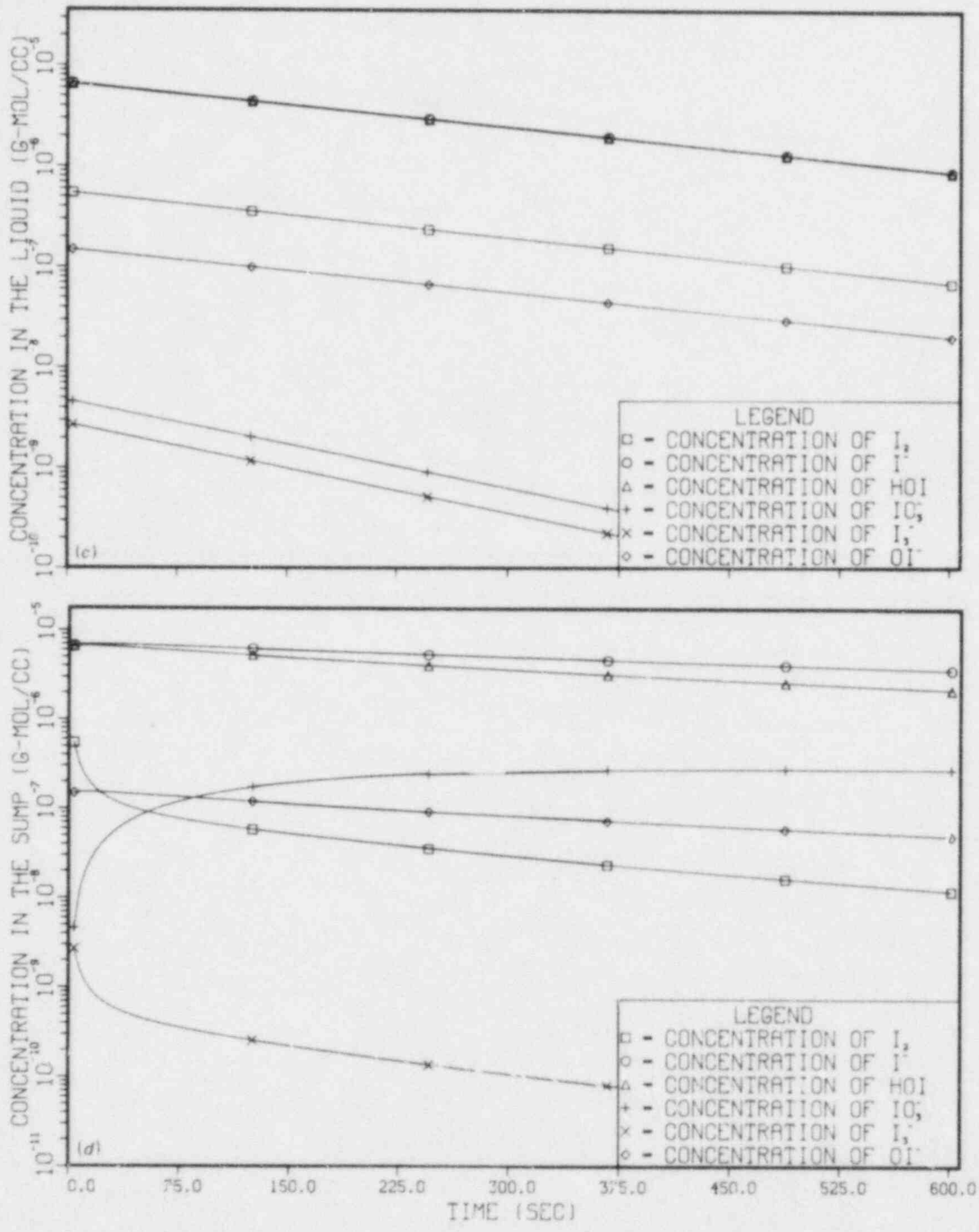

Fig. 31. (continued).

ORNL-DWG 84-6564 ETD (Part A)

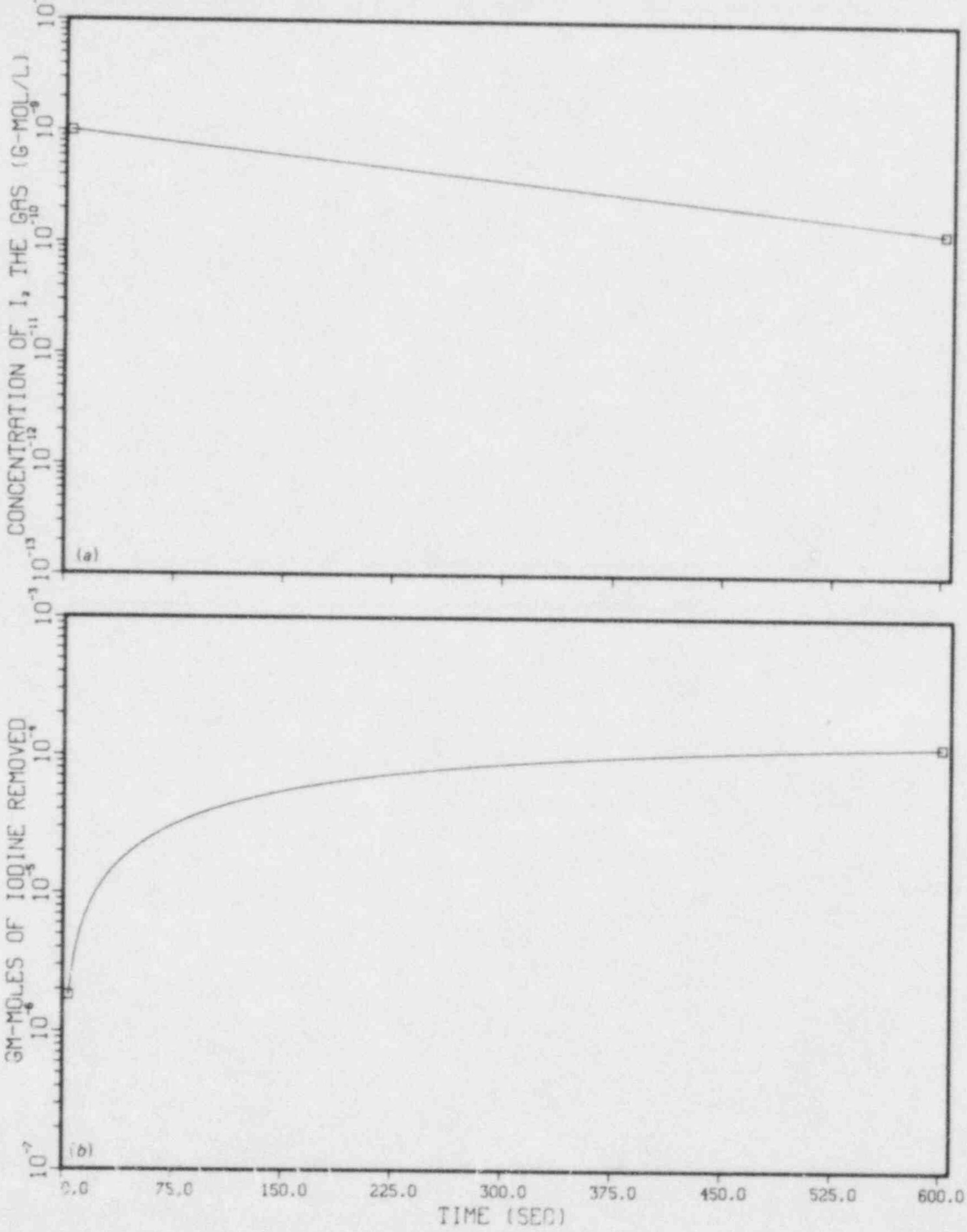

Fig. 32. Results of Spray Model. Initial concentration of molecular iodine in the gas phase of 1×10^{-9} moles/liter and a buffered pH of 9.0 in the liquid phase.

(a) Concentration of molecular iodine in the gas phase as a function of time.

(b) Number of moles of molecular iodine transferred as a function of time.

(c) Concentration of iodine species in the liquid drops as a function of time.

(d) Concentration of iodine species in the sump as a function of time.

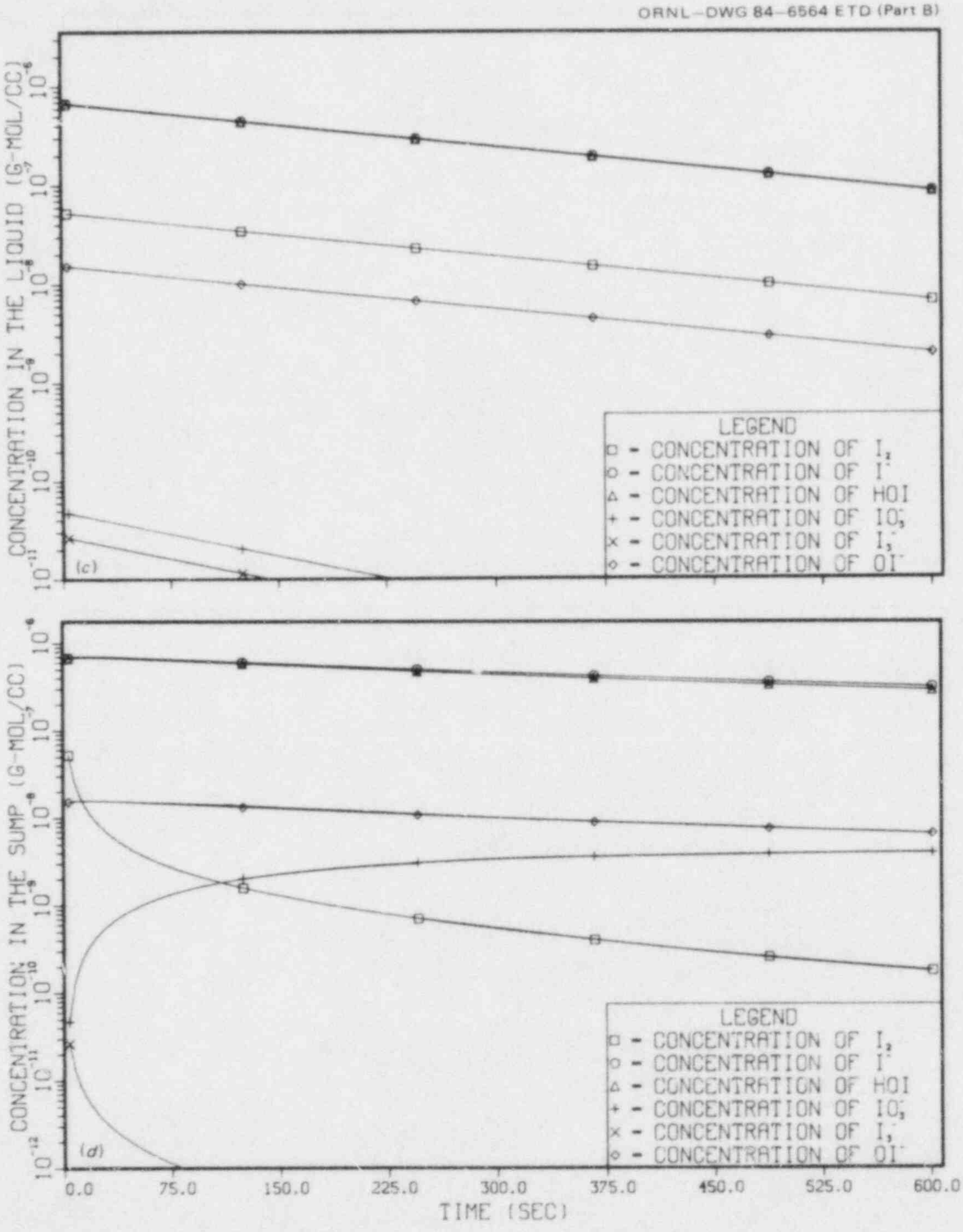

Fig. 32. (continued).

ORNL-DWG 84-6565 ETD (Part A)

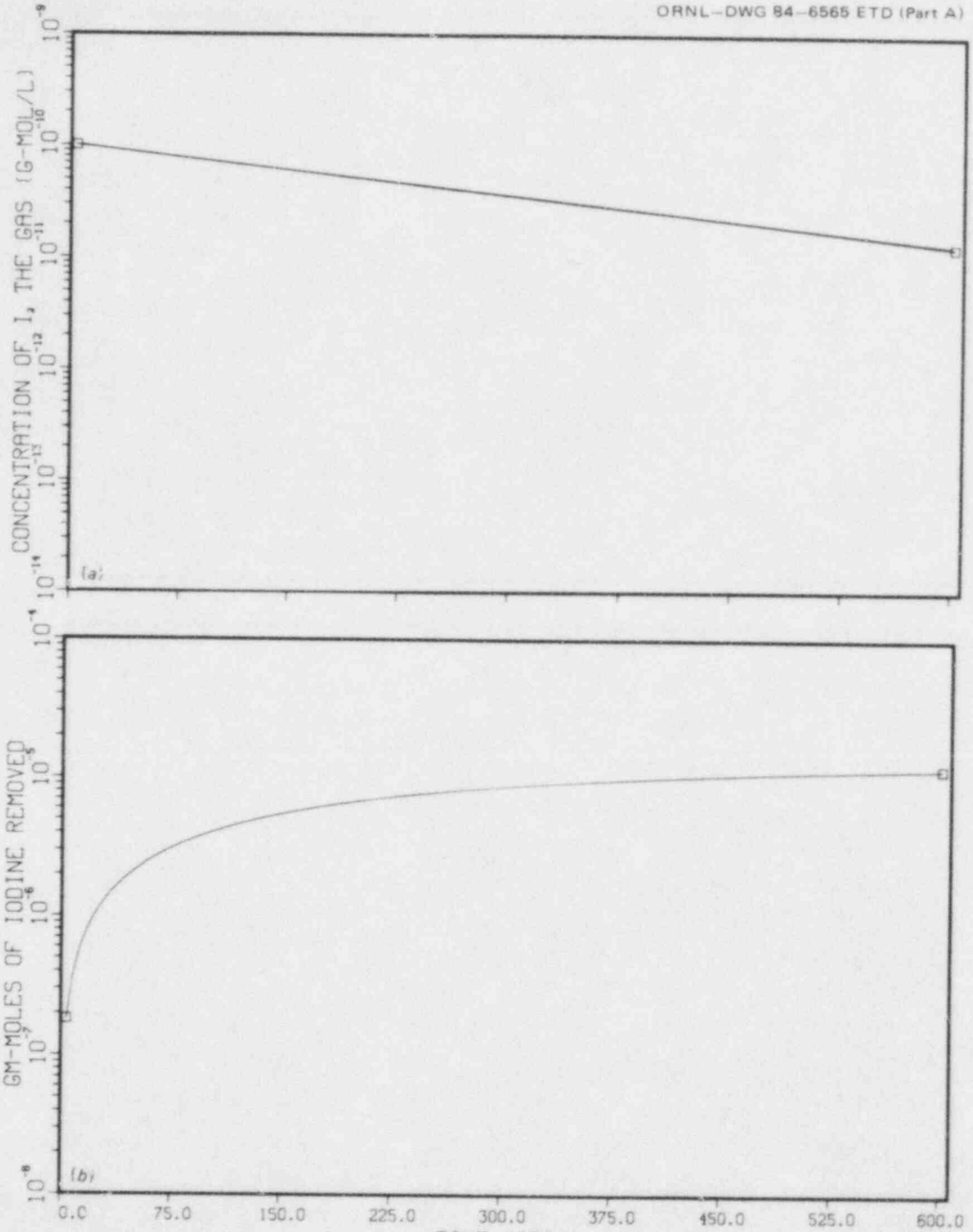

Fig. 33. Results of Spray Model. Initial concentration of molecular iodine in the gas phase of 1×10^{-10} moles/liter and a buffered pH of 9.0 in the liquid phase.

(a) Concentration of molecular iodine in the gas phase as a function of time.

(b) Number of moles of molecular iodine transferred as a function of time.

(c) Concentration of iodine species in the liquid drops as a function of time.

(d) Concentration of iodine species in the sump as a function of time.

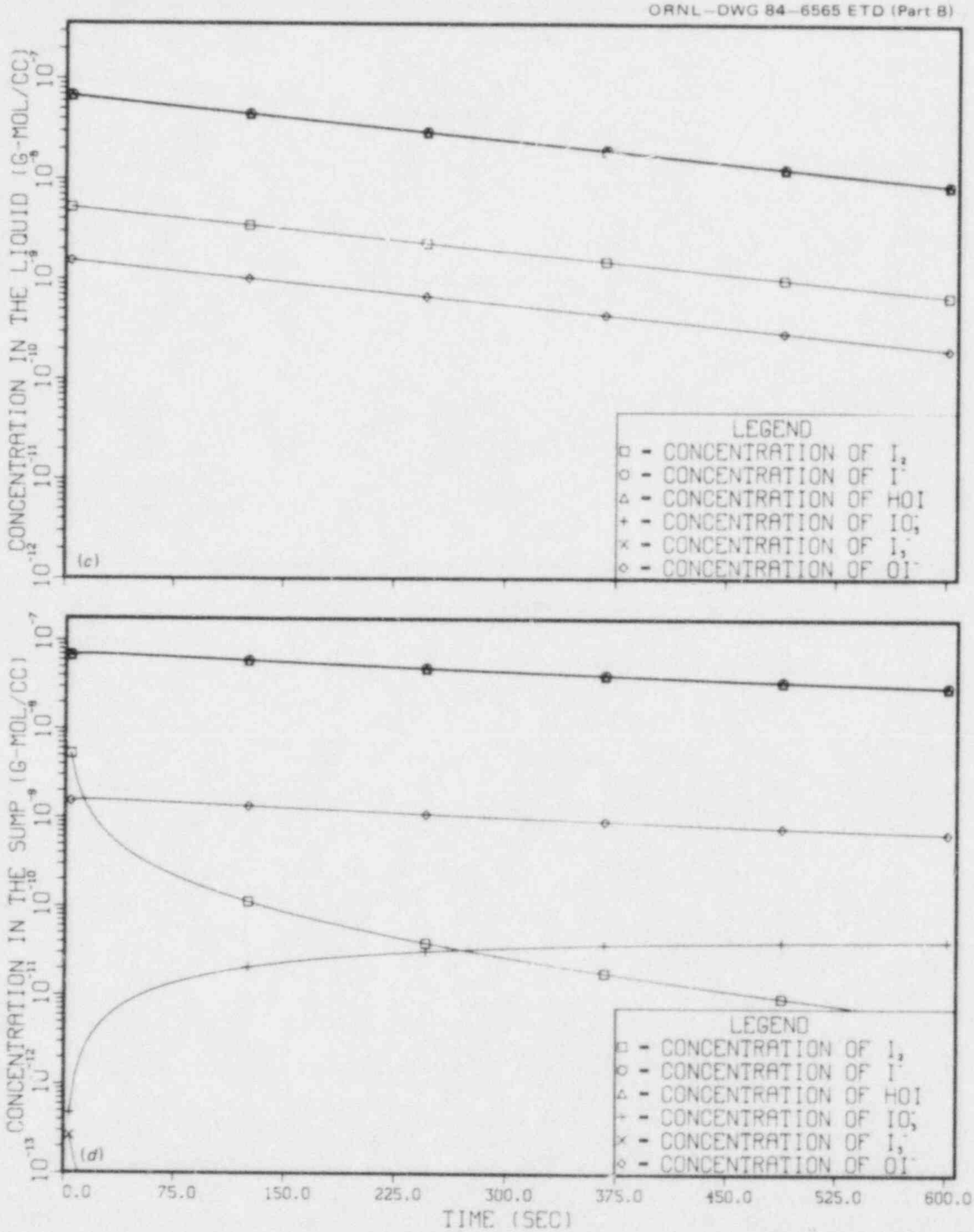

Fig. 33. (continued).

ORNL-DWG 84-6567 ETD (Part A)

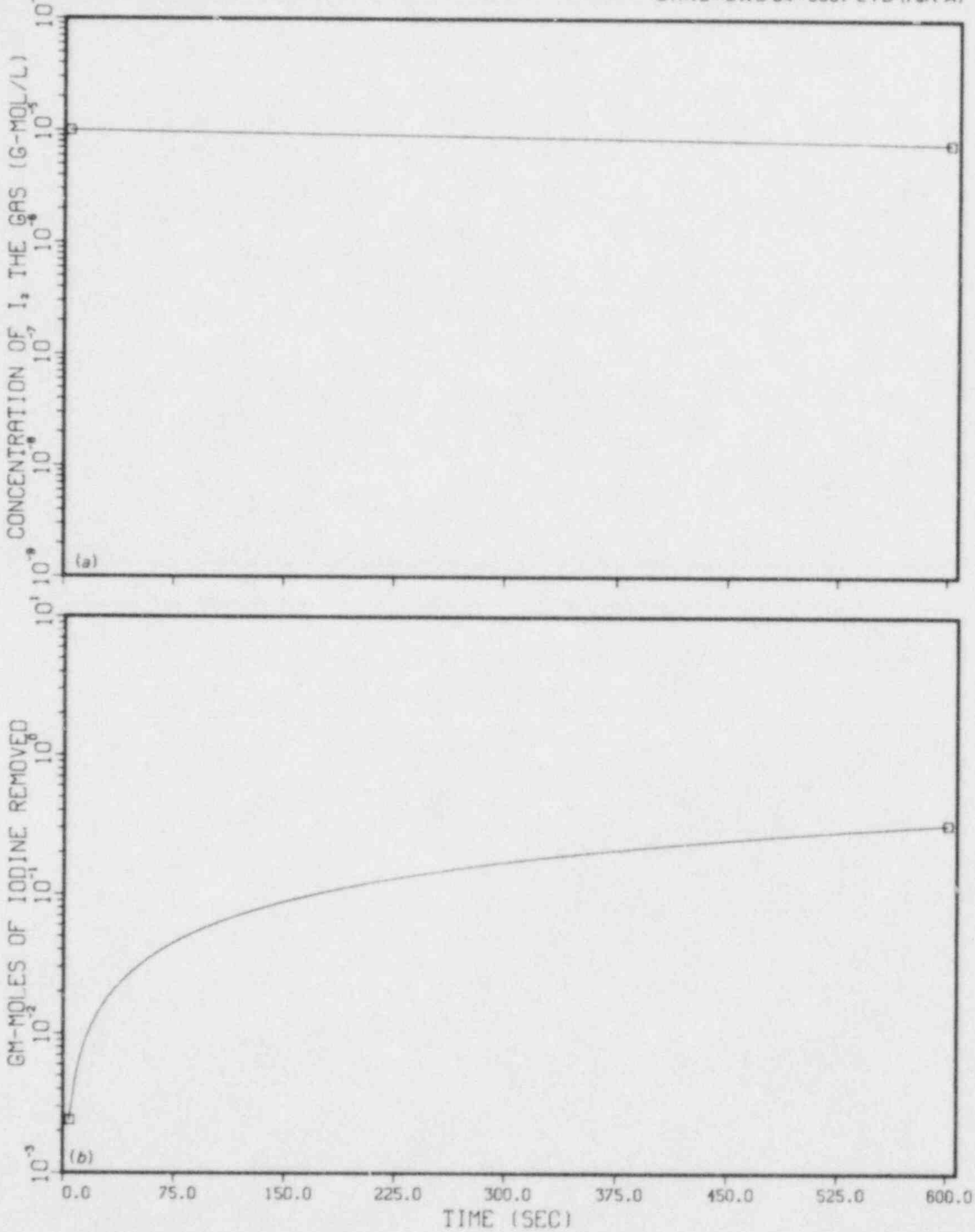

Fig. 34. Results of Spray Model. Initial concentration of molecular iodine in the gas phase of 1×10^{-5} moles/liter and a buffered pH of 7.0 in the liquid phase.

(a) Concentration of molecular iodine in the gas phase as a function of time.

(b) Number of moles of molecular iodine transferred as a function of time.

(c) Concentration of iodine species in the liquid drops as a function of time.

(d) Concentration of iodine species in the sump as a function of time.

ORNL-DWG 84-6567 ETD (Part B)

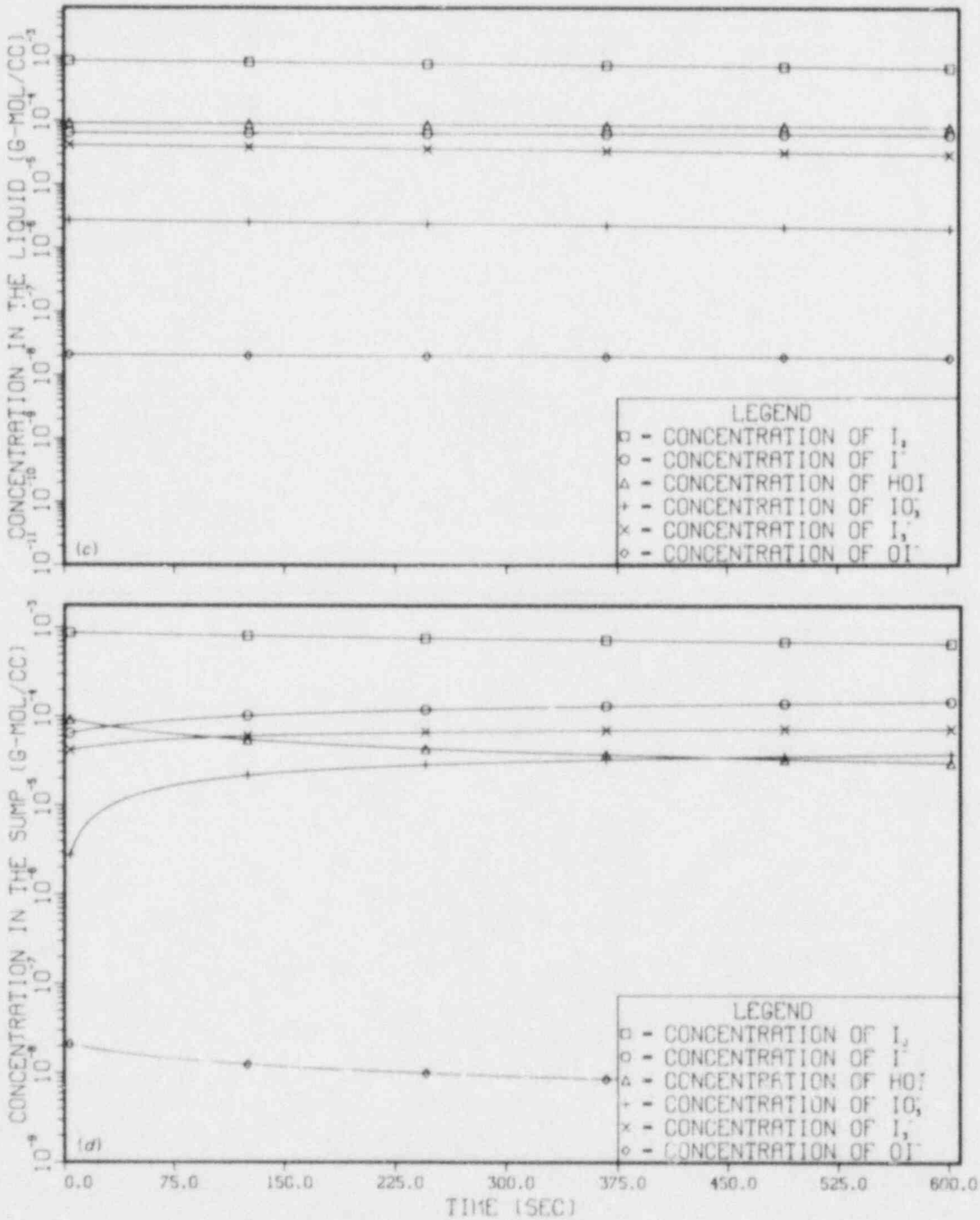

Fig. 34. (continued).

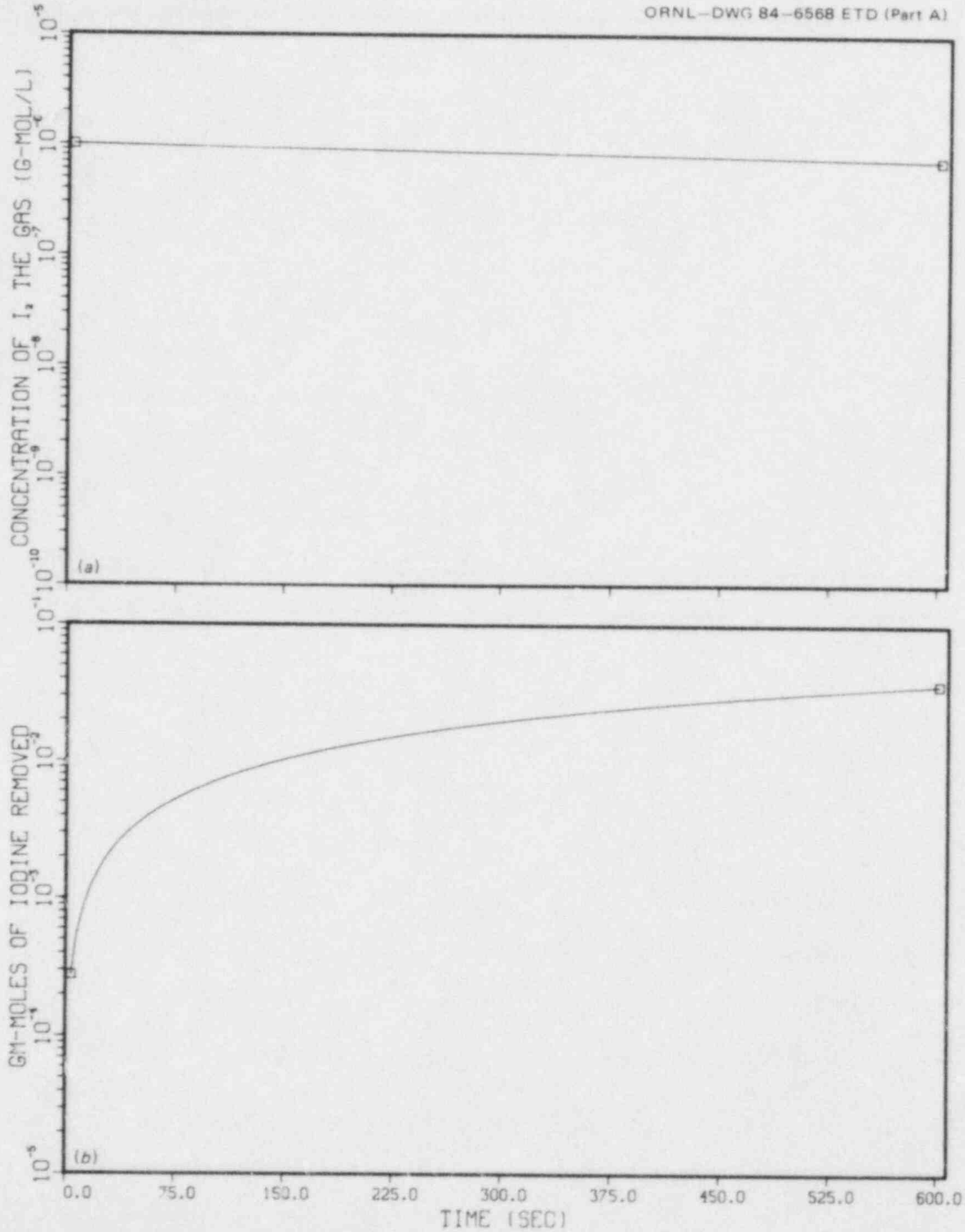

Fig. 35. Results of Spray Model. Initial concentration of molecular iodine in the gas phase of 1×10^{-6} moles/liter and a buffered pH of 7.0 in the liquid phase.

(a) Concentration of molecular iodine in the gas phase as a function of time.

(b) Number of moles of molecular iodine transferred as a function of time.

(c) Concentration of iodine species in the liquid drops as a function of time.

(d) Concentration of iodine species in the sump as a function of time.

ORNL-DWG 84-6568 ETD (Part B)

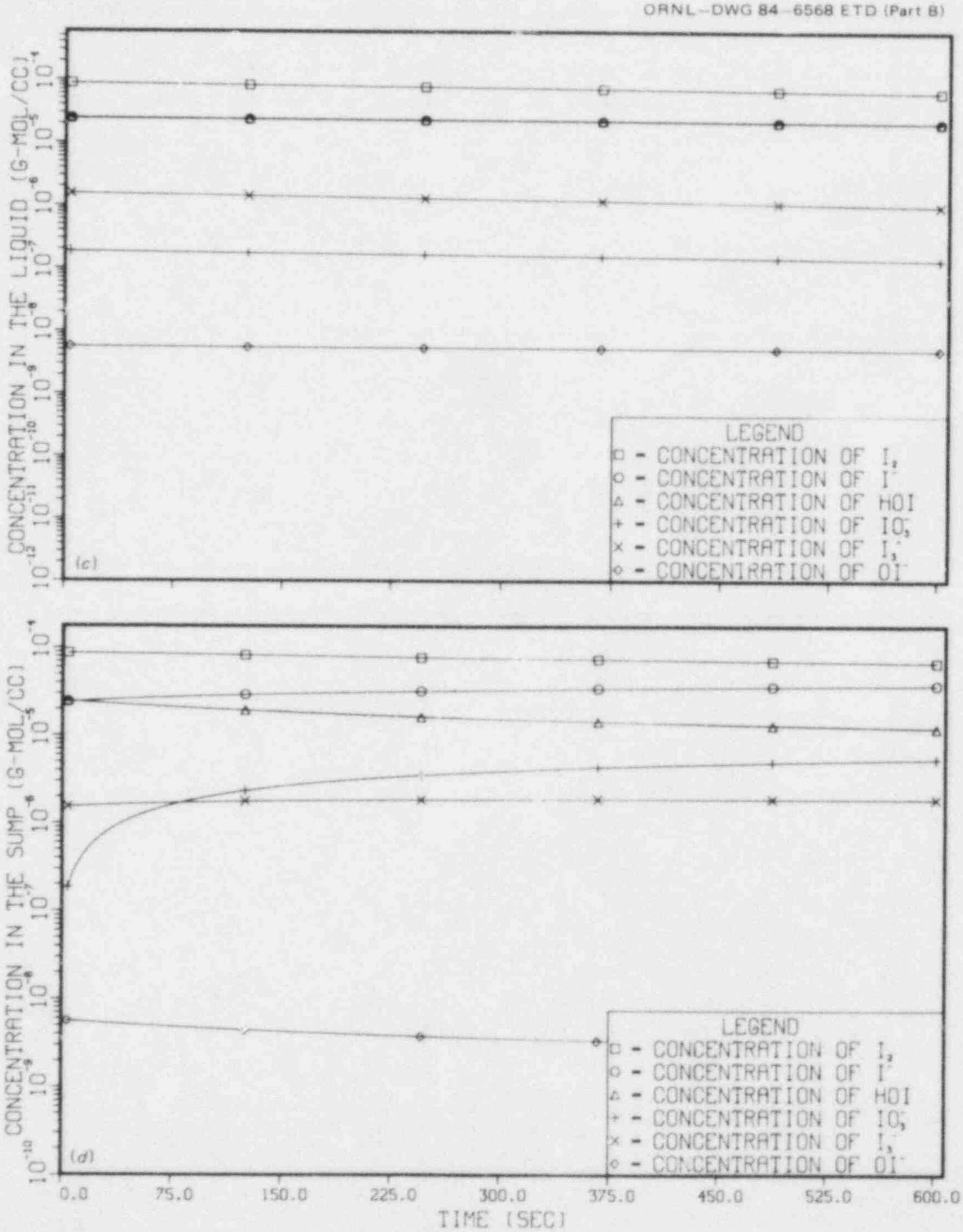

Fig. 35. (continued).

ORNL–DWG 84–6569 ETD (Part A)

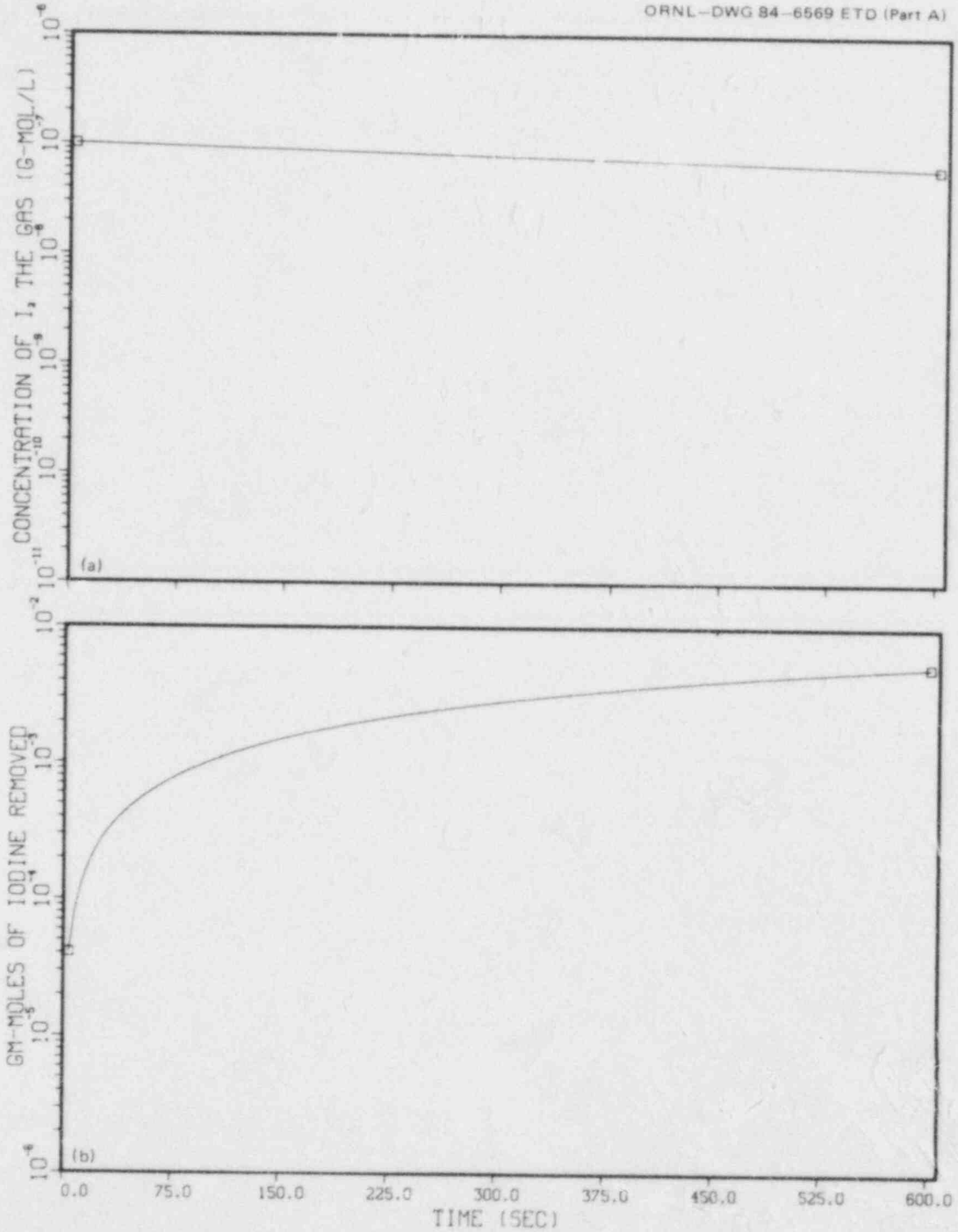

Fig. 36. Results of Spray Model. Initial concentration of molecular iodine in the gas phase of 1×10^{-7} moles/liter and a buffered pH of 7.0 in the liquid phase.

(a) Concentration of molecular iodine in the gas phase as a function of time.

(b) Number of moles of molecular iodine transferred as a function of time.

(c) Concentration of iodine species in the liquid drops as a function of time.

(d) Concentration of iodine species in the sump as a function of time.

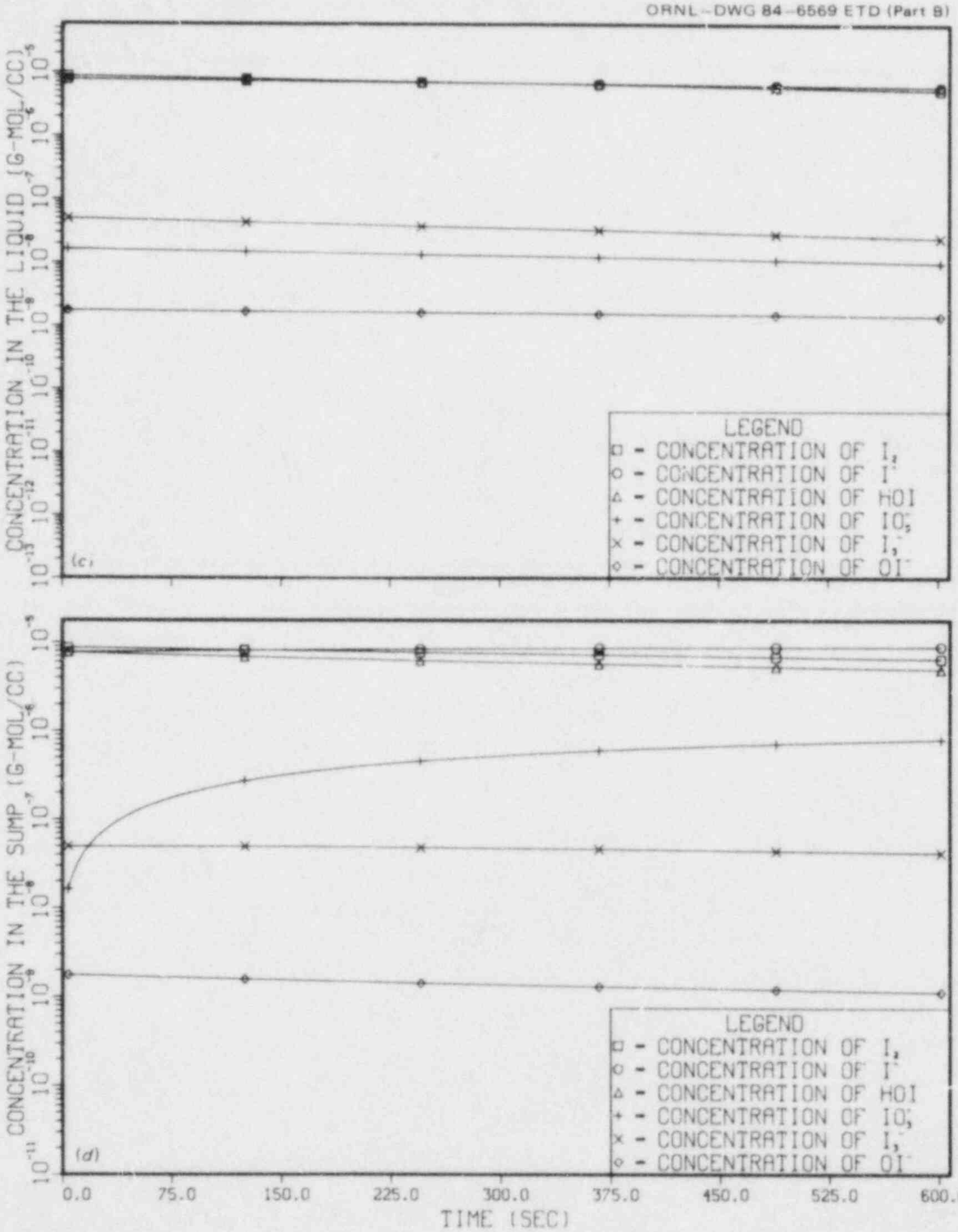

Fig. 36. (continued).

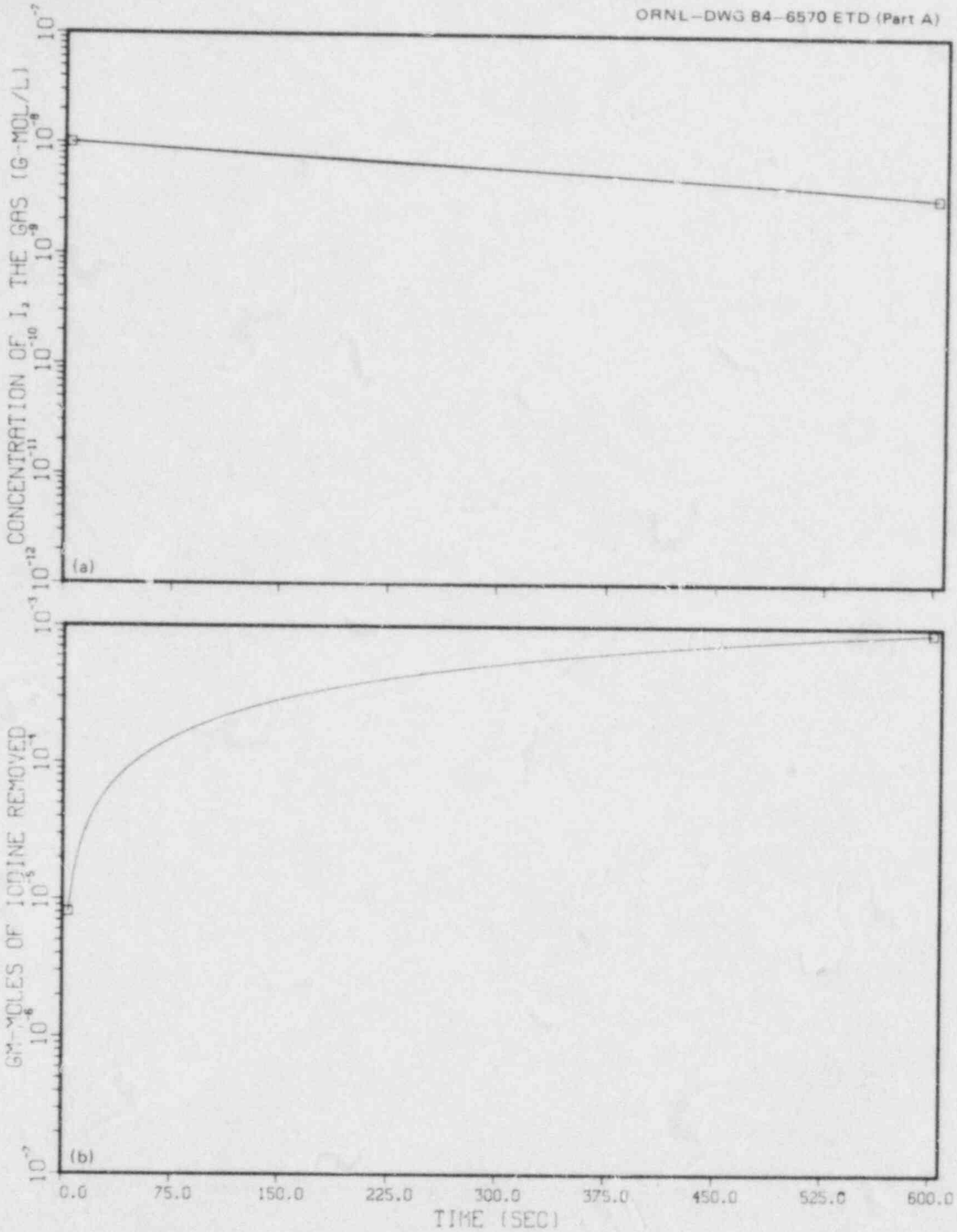

Fig. 37. Results of Spray Model. Initial concentration of molecular iodine in the gas phase of 1×10^{-8} moles/liter and a buffered pH of 7.0 in the liquid phase.

(a) Concentration of molecular iodine in the gas phase as a function of time.

(b) Number of moles of molecular iodine transferred as a function of time.

(c) Concentration of iodine species in the liquid drops as a function of time.

(d) Concentration of iodine species in the sump as a function of time.

ORNL-DWG 84-6570 ETD (Part B)

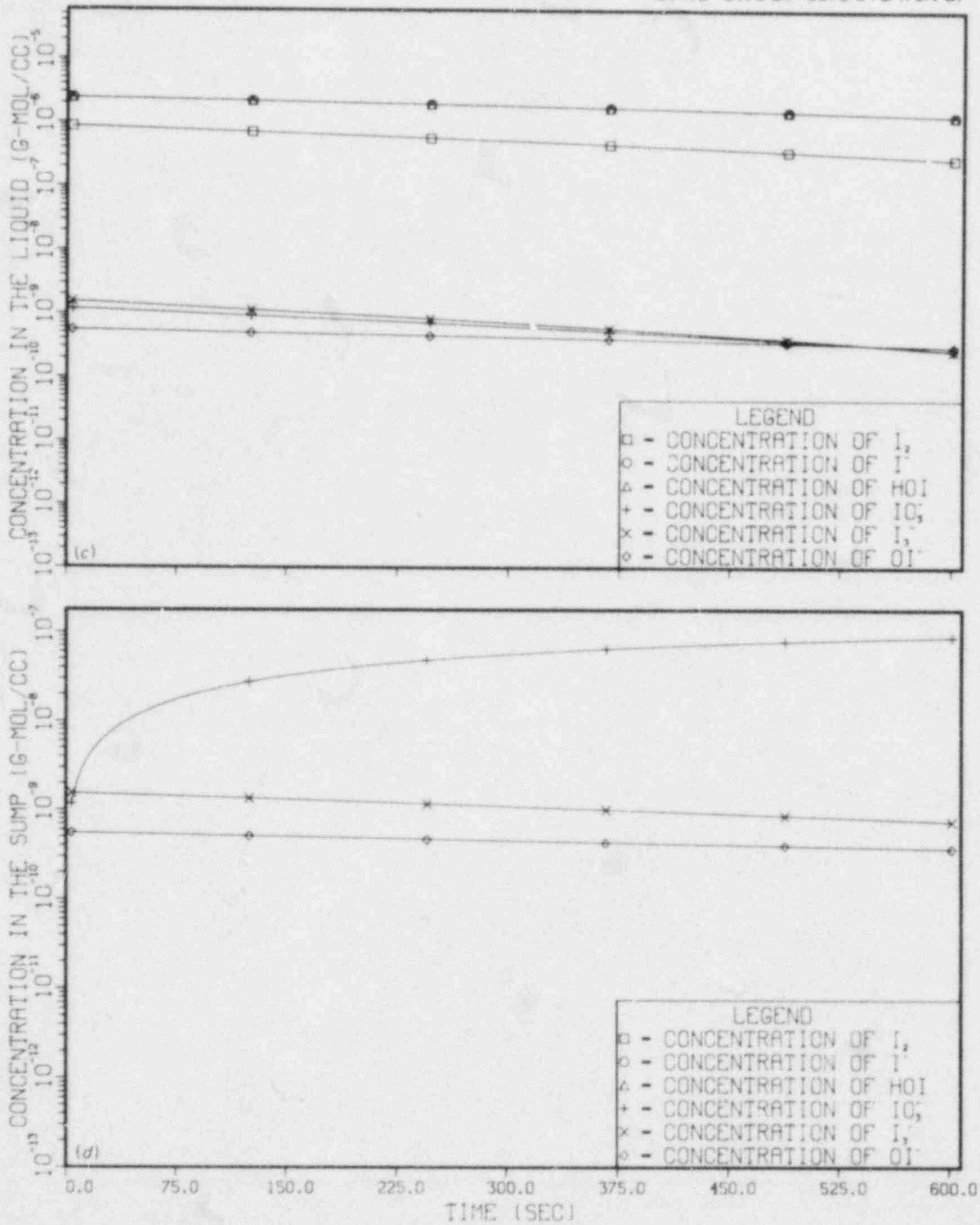

Fig. 37. (continued).

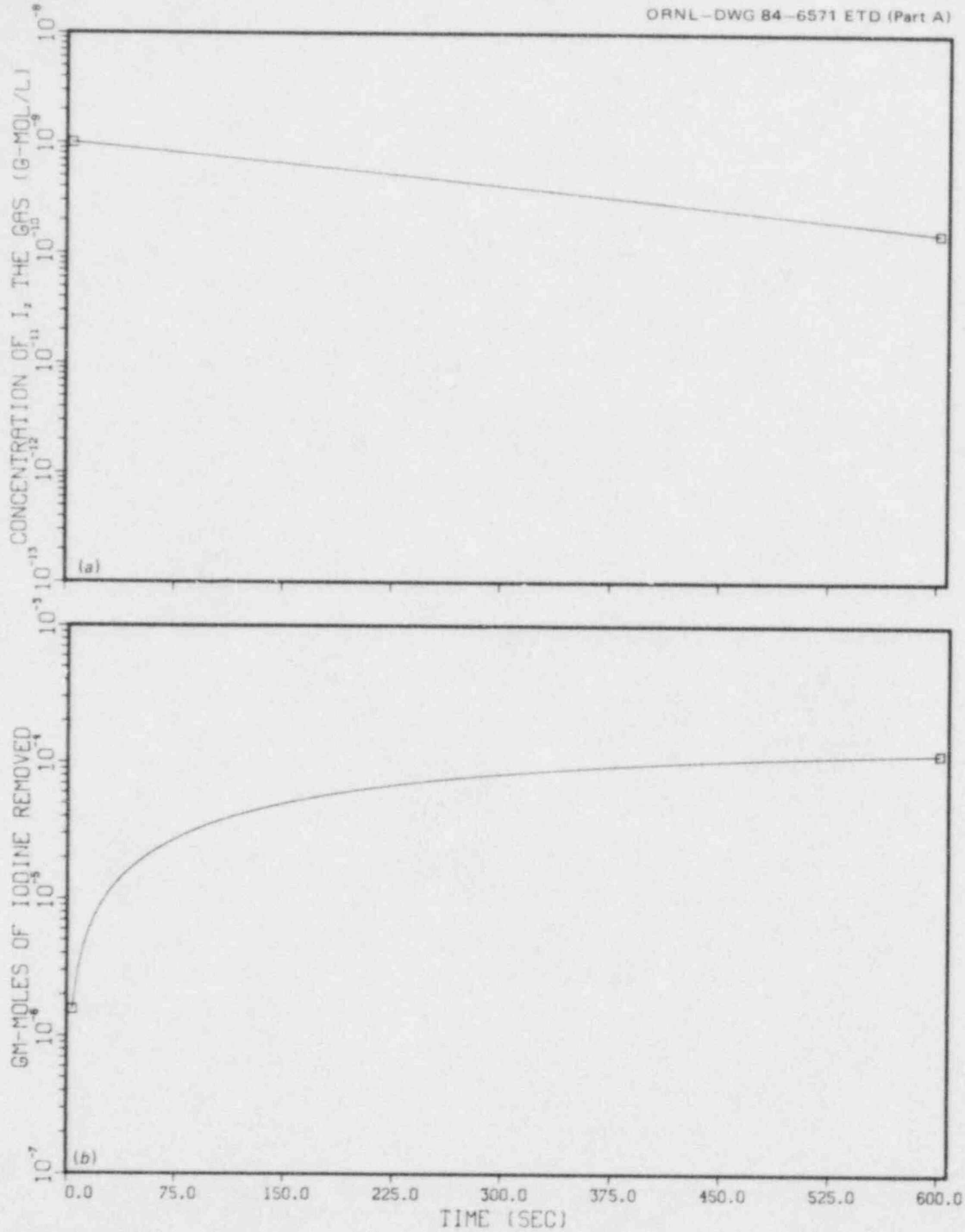

Fig. 38. Results of Spray Model. Initial concentration of molecular iodine in the gas phase of 1×10^{-9} moles/liter and a buffered pH of 7.0 in the liquid phase.

(a) Concentration of molecular iodine in the gas phase as a function of time.

(b) Number of moles of molecular iodine transferred as a function of time.

(c) Concentration of iodine species in the liquid drops as a function of time.

(d) Concentration of iodine species in the sump as a function of time.

ORNL–DWG 84–6571 ETD (Part B)

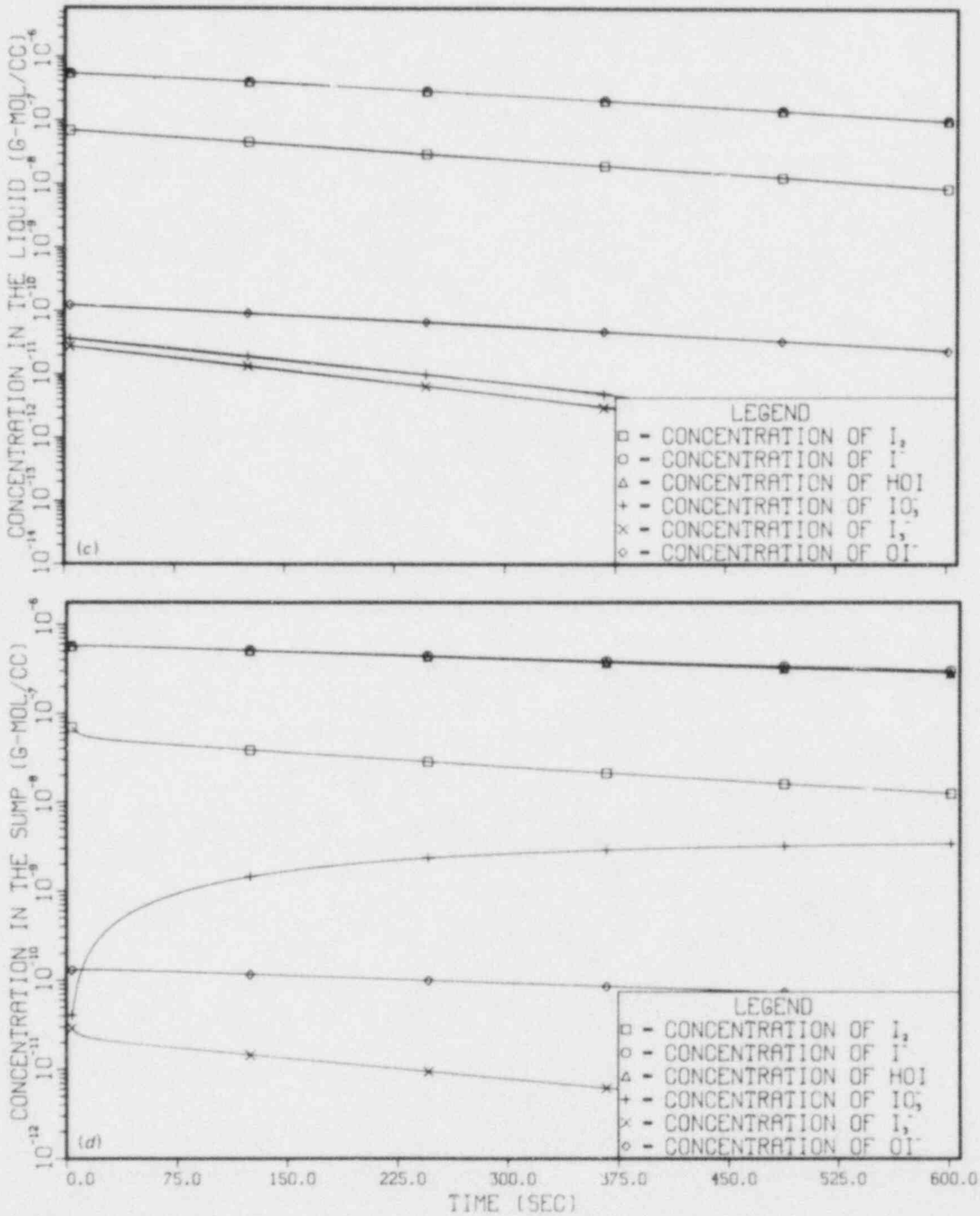

Fig. 38. (continued).

ORNL—DWG 84–6572 ETD (Part A)

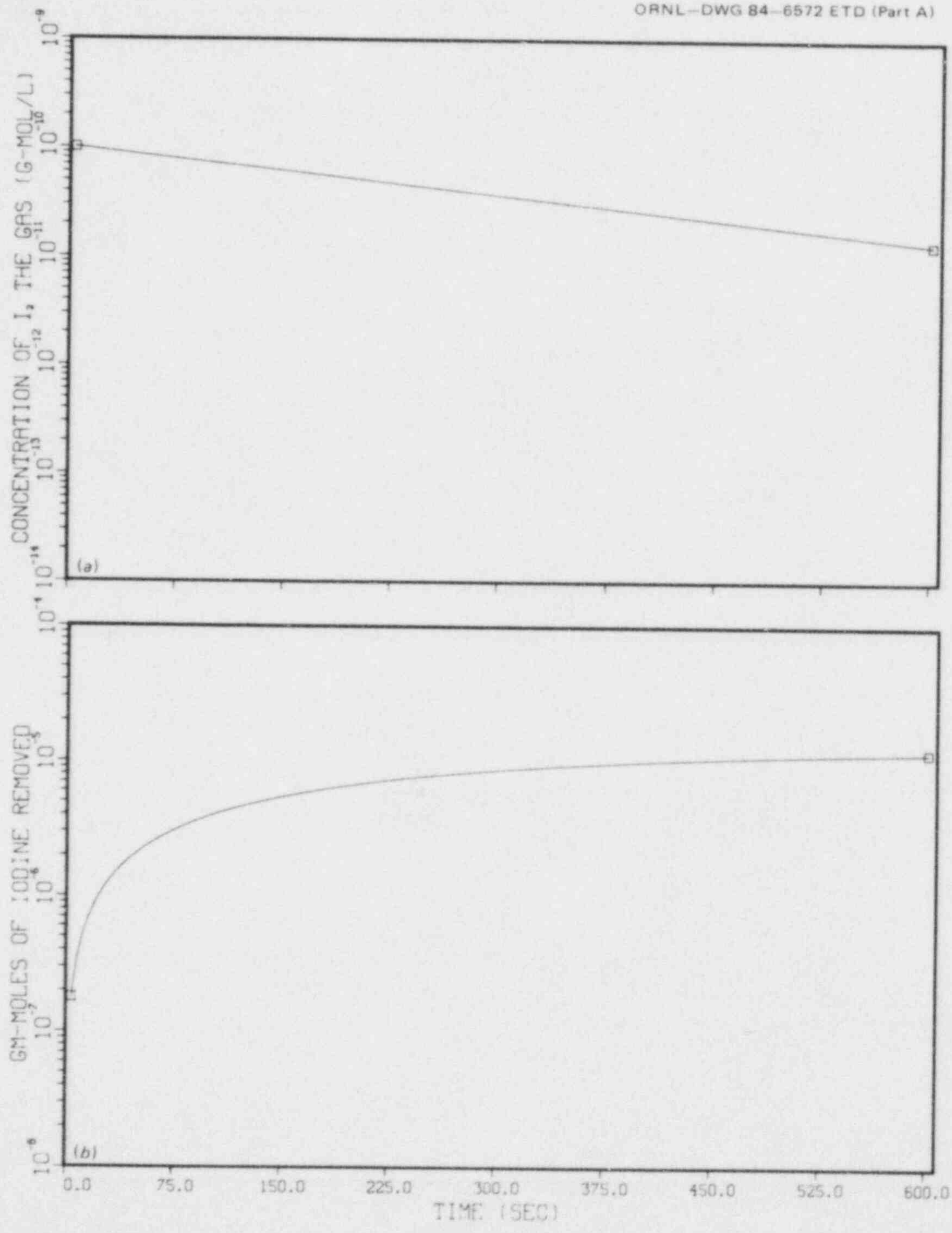

Fig. 39. Results of Spray Model. Initial concentration of molecular iodine in the gas phase of 1×10^{-10} moles/liter and a buffered pH of 7.0 in the liquid phase.

(a) Concentration of molecular iodine in the gas phase as a function of time.

(b) Number of moles of molecular iodine transferred as a function of time.

(c) Concentration of iodine species in the liquid drops as a function of time.

(d) Concentration of iodine species in the sump as a function of time.

ORNL-DWG 84-6572 ETD (Part B)

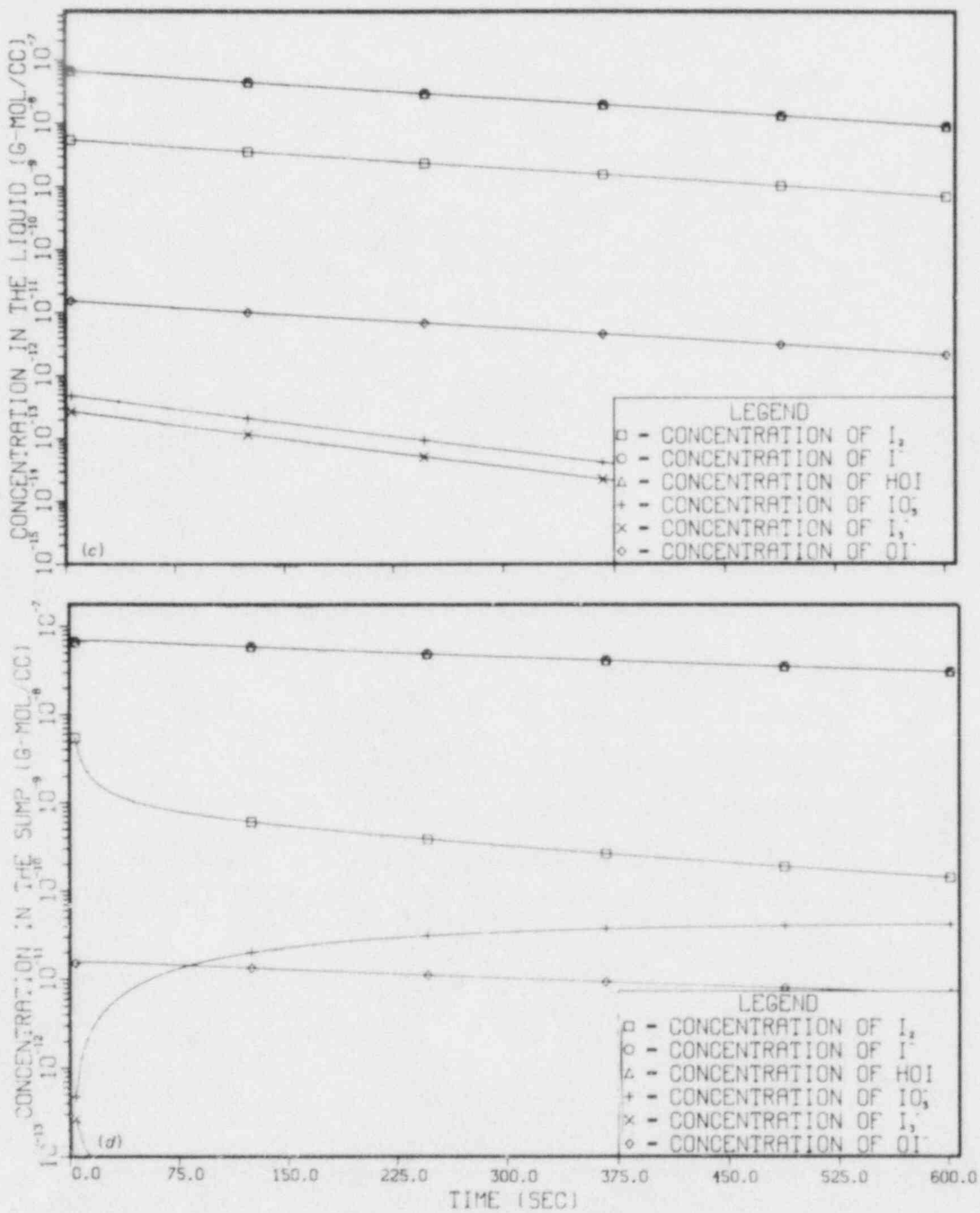

Fig. 39. (continued).

6. WALL-SPRAY MODEL

The wall-spray model calculates the removal of molecular iodine from the gas phase by a spray system and by contact with the wetted walls of the containment. This model incorporates the spray model to determine the removal by the sprays, and there is an additional falling liquid film routine to determine the removal of gaseous iodine by the walls that are wetted by the sprays. The vertical walls of the containment are cut into several horizontal cylindrical pieces in which molecular iodine is absorbed by the water flowing down the walls. The effect of variation in width is neglected within each cylindrical piece, and then the molecular iodine is reacted with the water in each piece. The height of each piece or section of the wall is determined by the drop exposure time and the velocity of the water on the walls. For this model, the percentage of water that flows down the walls must be known or estimated.

The assumptions for the wall-spray model are exactly those for the spray model plus assumptions for the wall. These assumptions are:

1) each drop has a completely mixed bulk liquid,
2) resistance to mass transfer exists in both the gas phase and the liquid phase,
3) the only species which transfers (has volatility) in or out of the drop is molecular iodine (I_2),
4) reactions occur in the bulk of the liquid,
5) each drop falls at its terminal velocity,
6) every drop falls the same height,
7) each drop, at all times, has a constant surface area and constant volume,
8) there are no interactions between drops,
9) for the lifetime of a drop, the gas phase remains constant but the gas phase concentration can change slowly over several drop lifetimes,
10) there is no transfer of heat or water between the drop and the gas phase (see Chapter 4, DROP MODEL),
11) the fluid in each cylindrical piece or slice of the wall is well mixed,
12) reactions occur in the bulk liquid of each slice,
13) water only enters on the wall at the top, and
14) water only exits the wall at the bottom where it runs into a sump.

The boundary conditions for the wall are defined at the extremes of the y and x coordinates as defined on Figure 40, and are as follows:[6]

1) at $y = 0$ and at all values of x, the concentration of molecular iodine equals the concentration of molecular iodine in the liquid drop when it strikes the wall,
2) at $x = 0$ and at all values of y, the concentration of molecular iodine in the liquid on the wall is equal to the interphase equilibrium concentration of molecular iodine in the gas, and
3) at $x = \delta$ and at all values of y, $\partial[I_2]/\partial x = 0$, (assume no diffusion into the wall).

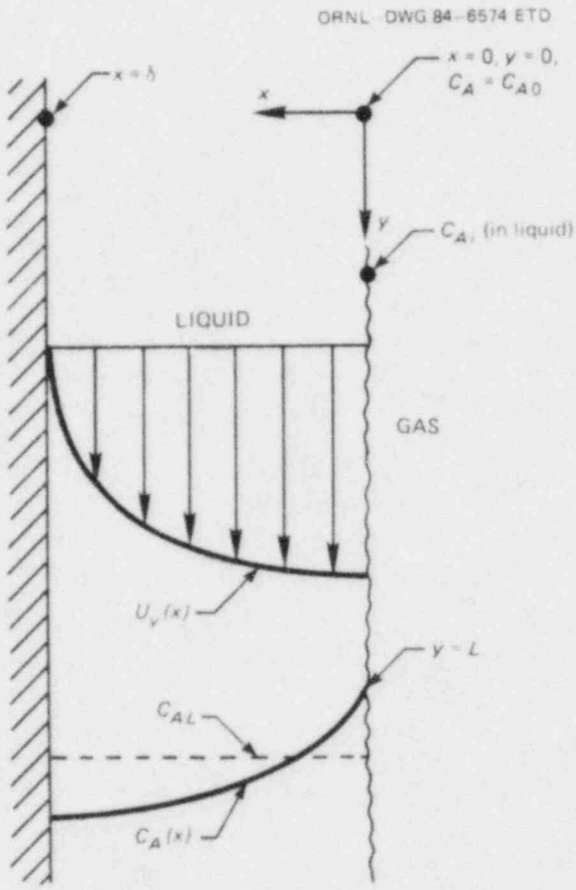

Fig. 40. Boundary Conditions for Falling Liquid Film.

The calculations for mass transfer to a falling liquid film are outlined in Treybal.[6] One assumption in the outline by Treybal[6] is that no chemical reactions occur in the liquid. The concentration profile, $C_A(x)$ (shown in Figure 40), is non-linear in shape (slope is a function of the distance from the interface). The mass transfer coefficient is proportional to the slope of the concentration profile at the interface. The local mass transfer rate can be expressed by:

$$N_A = - D_l \left(\frac{\partial C_A}{\partial x}\right)_{x=0} = k_l \, (C_{Ai} - \overline{C}_{A,L}) \tag{58}$$

where

N_A = mass transfer flux across the interface of species A,

D_l = diffusivity of the transferring species in the liquid,

$\left(\frac{\partial C_A}{\partial x}\right)_{x=0}$ = concentration profile of the transferring species in the x direction,

k_l = local mass transfer coefficient, and

$\overline{C}_{A,L}$ = average bulk concentration of the transferring species after the water on the walls has Fallen a distance L, the height of each horizontal piece.

When reactions occur in the liquid, the concentration profile, in the liquid will change. This will change the mass transfer coefficient in the liquid. Therefore, the assumption that the reactions induce a small error in the wall film mass transfer rate is made. However, since the transfer to the wall is only a small fraction of the total iodine absorption, small errors in this part of the wall-spray model will be insignificant. A more elaborate simulation of the transfer of iodine to the falling liquid film is not justified.

The average mass transfer flux for the wall liquid film, $N_{a,w}$, is defined as:[6]

$$N_{a,w} = k_{l,av} ([I_2^i] - [I_{2,B}])_M = \frac{u_y \delta}{H} ([I_{2,B}^l] - [I_2^o]) \quad (59)$$

where

$k_{l,av}$ = the average liquid mass transfer coefficient,

$[I_2^i]$ = the concentration of molecular iodine at the interface,

$[I_{2,B}^l]$ = concentration of molecular iodine at the bottom of the wall,

$[I_{2,B}]$ = the average bulk concentration of molecular iodine,

$[I_2^o]$ = the initial concentration of molecular iodine in the liquid,

u_y = average velocity of the liquid down the wall,

δ = liquid thickness on the wall,

H = wall height, and

$([I_2^i] - [I_{2,B}])_m$ = logarithmic average concentration gradient.

Valves for $k_{l,av}$ and for the other parameters can be obtained as follows:[6]

$$k_{l,av} = (6\ D_l\ \Gamma/\pi\ \rho_l \delta\ H)^{1/2}\ , \quad (60)$$

Γ = mass rate of flow,

π = 3.1415... ,

ρ_l = density of water,

$$\delta = (3\,\mu_1 \Gamma/\rho_1^2\, g)^{1/3} \;, \tag{61}$$

g = acceleration of gravity,

μ_1 = viscosity of water,

$$u_y = (\Gamma/\rho_1 \delta) \;, \text{ and} \tag{62}$$

$$([I_2^i] - [I_{2,B}])_M = \frac{([I_2^i] - [I_2^o]) - ([I_2^i] - [I_{2,B}^1])}{\mathrm{Ln}\;(([I_2^i] - [I_2^o])/([I_2^i] - [I_{2,B}^1]))} \;. \tag{63}$$

Equation (59) can be solved by iterating for $[I_2^1,B]$:

$$k_{1,av}\,\frac{(([I_2^i] - [I_2^o]) - ([I_2^i] - [I_{2,B}^1]))}{\mathrm{Ln}(([I_2^i] - [I_2^o)/(I_2^i] - [I_{2,B}^1]))} = \frac{u_y\,\delta}{H}\,([I_{2,B}^1] - [I_2^o]) \;. \tag{64}$$

Since all variables are known except for $[I_{2,B}^1]$, one can iterate for $[I_{2,B}^1]$, the concentration of molecular iodine at the bottom of each segment. Once $[I_{2,B}^1]$ is known, one can calculate the moles of molecular iodine transferred to the drop.

The algorithm for the wall spray model is (see Figure 41 for Wall-Spray Model Flowsheet):

1) determine all physical properties ı r the gas and liquid phases for both the spray and the wall section,
2) determine the number of loops, N, for the spray section of the program,
3) determine the number of pieces into which the wall will be broken,
4) determine the total surface areas and total volumes for the drops and for a wall slice,
5) execute the drop model until the drop reaches the wall,
   a) determine the number of moles of molecular iodine that are transferred to the large drop from the gas phase,
   b) calculate the concentration of molecular iodine in the large liquid drop,
   c) determine the concentration of all species in the large liquid drop due to the iodine hydrolysis reactions,
6) store the concentration of the drop (to be used as the initial concentration of the liquid of the wall),
7) continue execution of the drop model until the drop has reached the fall height,
8) execute the wall model for each section used to represent the wall,
9) execute the kinetic model on the liquid in the sump,

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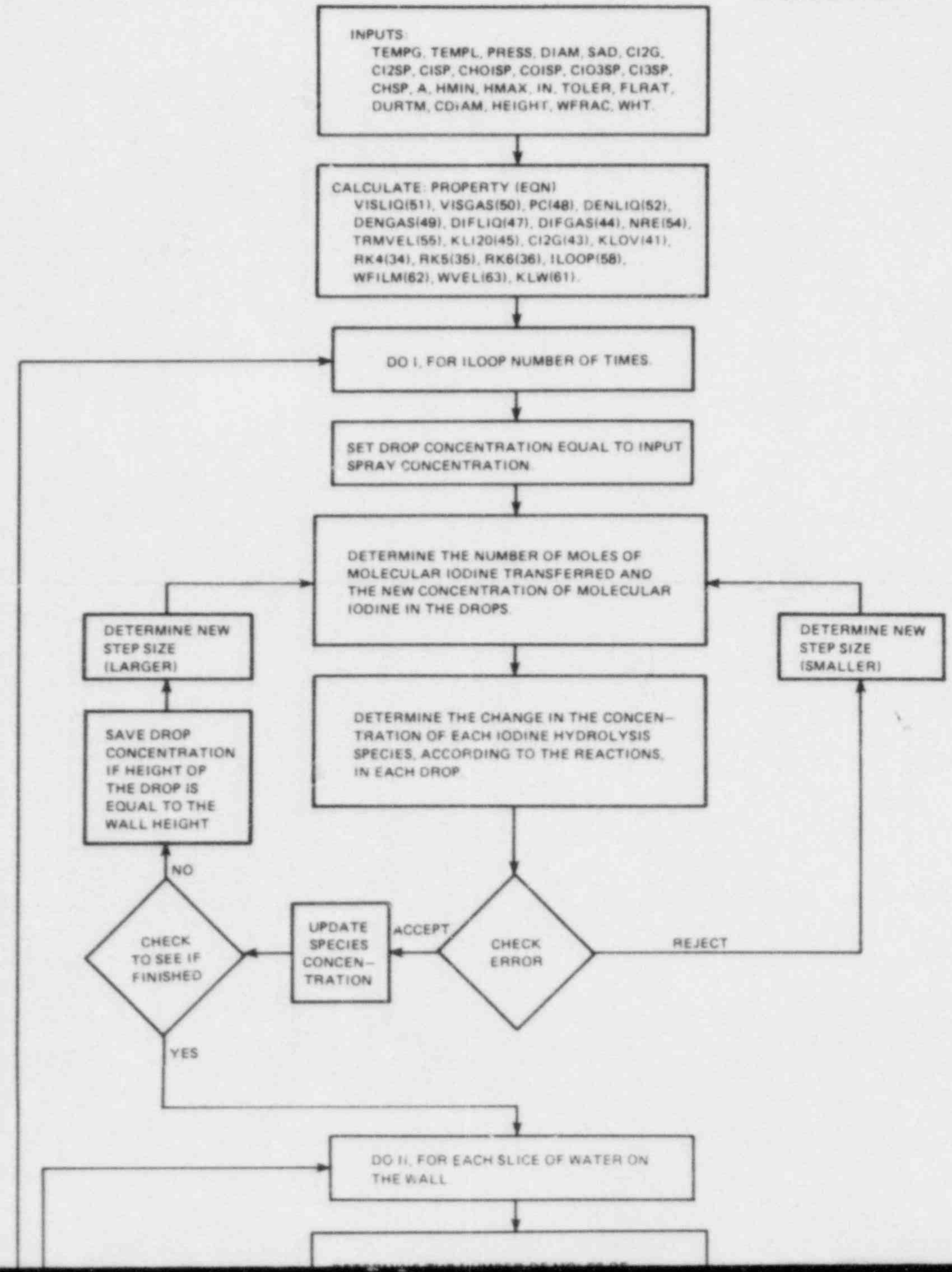

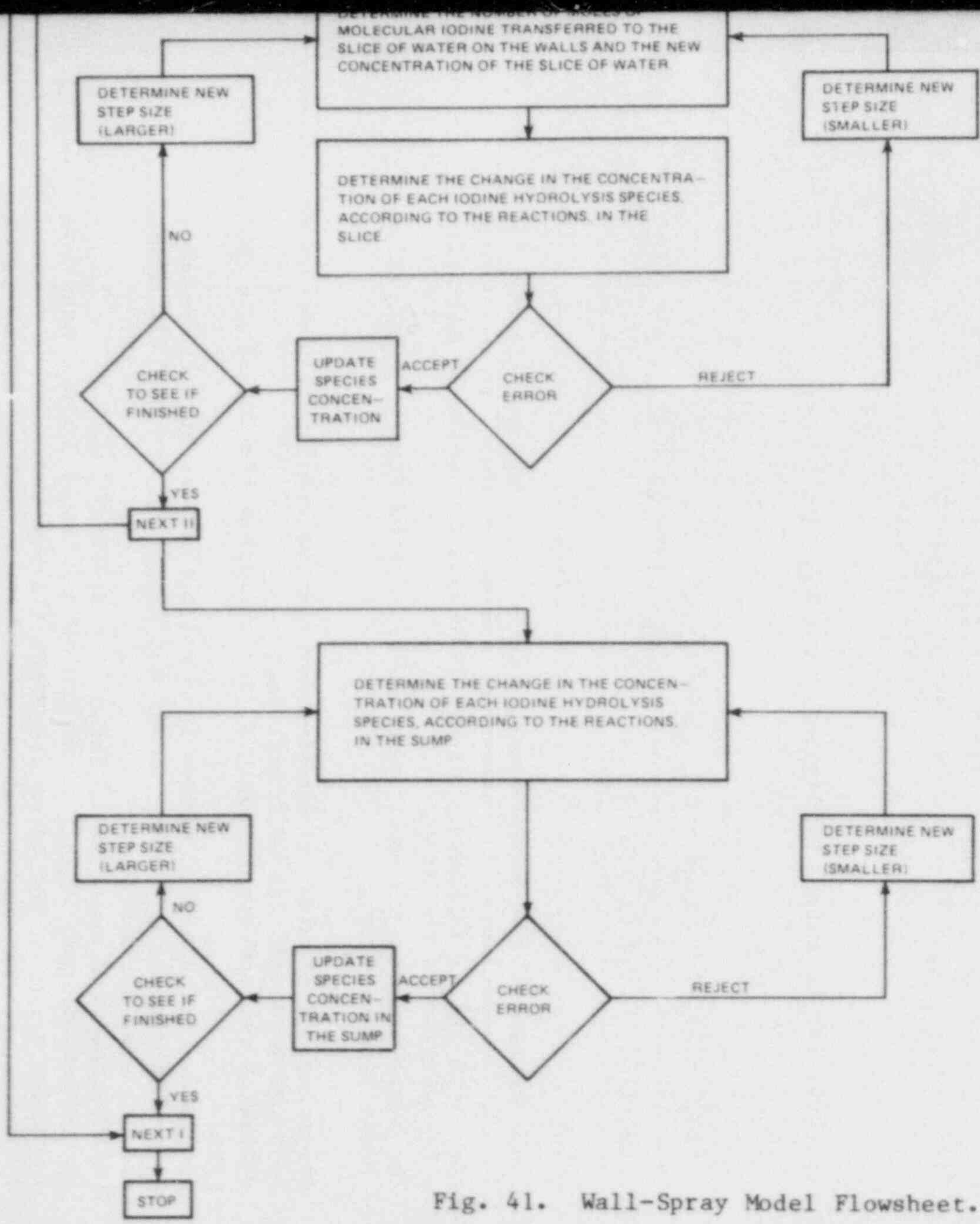

Fig. 41. Wall-Spray Model Flowsheet.

10) determine the total number of moles of molecular iodine transferred to the liquid and calculate the new gas phase concentration,
11) loop back to 5) until the spray part of the model is finished,
12) execute the wall model on the water that remains on the wall,
13) execute the kinetic model on the liquid in the sump,
14) determine the total number of moles removed and the new gas phase concentration of molecular iodine and,
15) loop back number to 12 until all of the water has flowed off the wall.

A FORTRAN program with this algorithm is shown in Appendix F.

Input parameters for this model are the same as those for the spray model with the addition of two more parameters for the wall section of the model. The inputs are:

1) initial gas phase concentration of molecular iodine,
2) initial liquid phase concentration of all iodine hydrolysis species,
3) whether buffered or unbuffered,
4) temperature of both gas and liquid phases
5) pressure,
6) average drop surface area diameter,
7) average drop volume diameter,
8) spray time,
9) spray flow rate,
10) drop fall height,
11) containment diameter,
12) relative error control (see Appendix A, Numerical Technique),
13) percentage of spray flow rate which flows down the wall, and
14) height of the wall.

A series of computer runs were performed for initial concentrations of molecular iodine in the gas phase of 1.0×10^{-7} to 1.0×10^{-10} moles/liter for 10 minute spray times for and a buffered pH valves of 9; the results are shown is Figures 42 to 43. The specific input parameters used for these runs are:

1) initial liquid phase concentrations are all zero except for the hydrogen ion concentration,
2) all spray solutions are buffered,
3) temperature of the gas is 298K and the temperature of the liquid is 298K,
4) pressure is 1 atmosphere,
5) drop surface area diameter is 0.1 centimeters,
6) drop volume diameter is 0.1 centimeter,
7) spray time is 10 minutes,
8) spray flow rate is 37 liters/minute,
9) drop fall height is 15.4 meters,
10) containment diameter is 3.3 meters,
11) the percentage of spray that flows down the wall is 5%, and
12) the wall height is 3.3 meters.

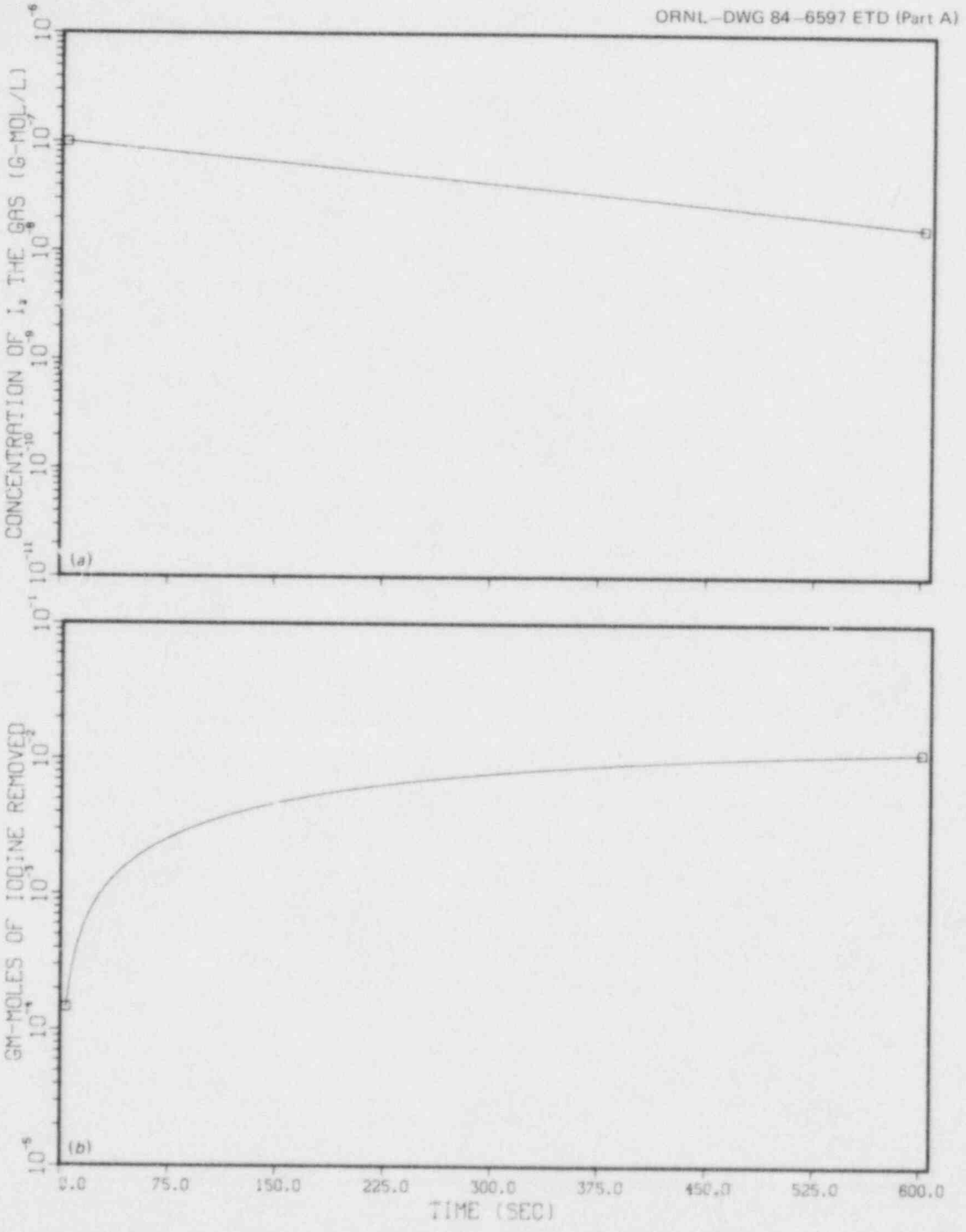

Fig. 42. Results of Wall-Spray Model. Initial concentration of molecular iodine in the gas phase of 1×10^{-7} moles/liter and a buffered pH of 9.0 in the liquid phase.

(a) Concentration of molecular iodine in the gas phase as a function of time.

(b) Number of moles of molecular iodine transferred as a function of time.

(c) Concentration of iodine species in the liquid drops as a function of time.

(d) Concentration of iodine species in the sump as a function of time.

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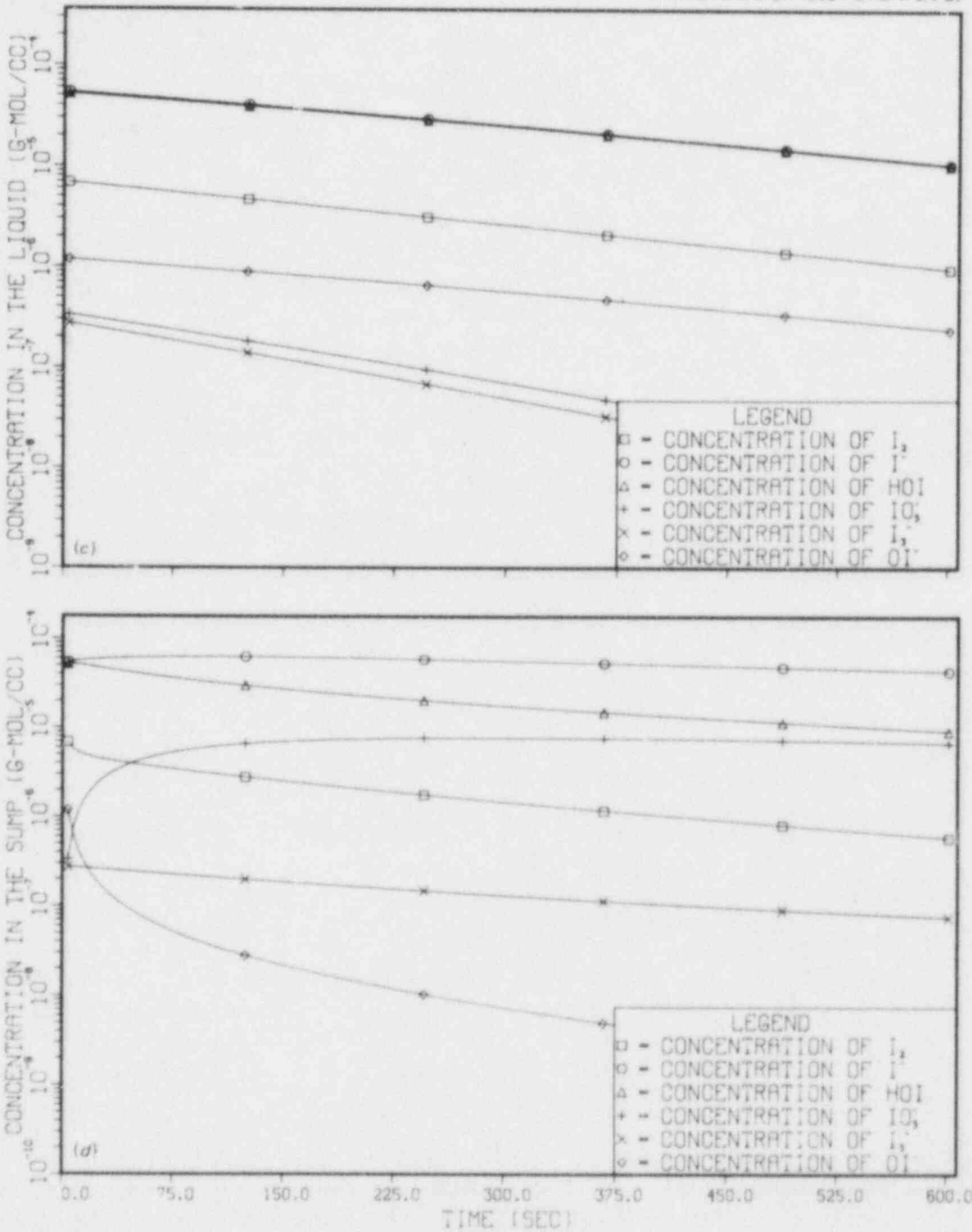


Fig. 42. (continued).

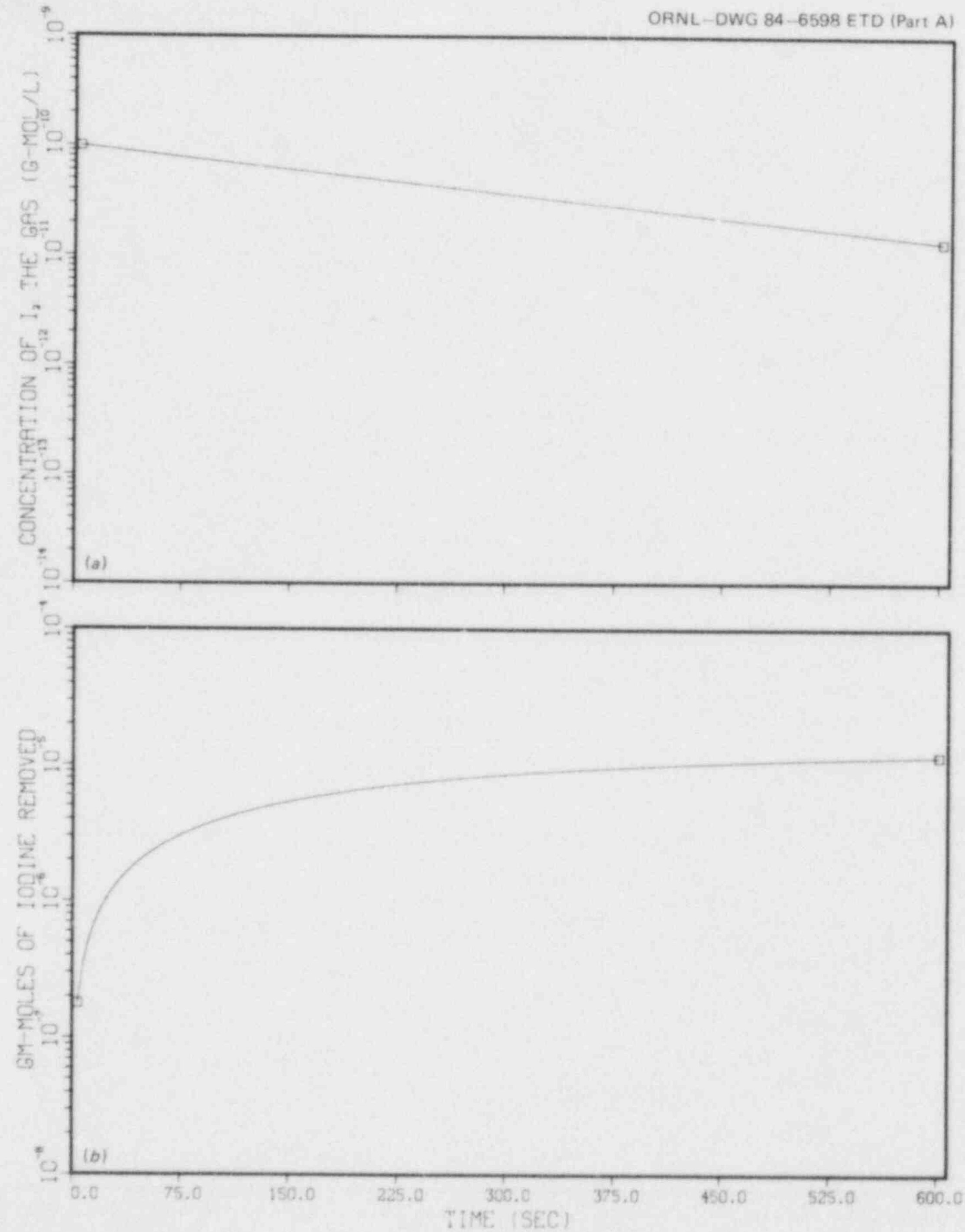


Fig. 43. Results of Wall-Spray Model. Initial concentration of molecular iodine in the gas phase of 1×10^{-10} moles/liter and a buffered pH of 9.0 in the liquid phase.

(a) Concentration of molecular iodine in the gas phase as a function of time.
(b) Number of moles of molecular iodine transferred as a function of time.
(c) Concentration of iodine species in the liquid drops as a function of time.
(d) Concentration of iodine species in the sump as a function of time.

ORNL-DWG 84-6598 ETD (Part B)

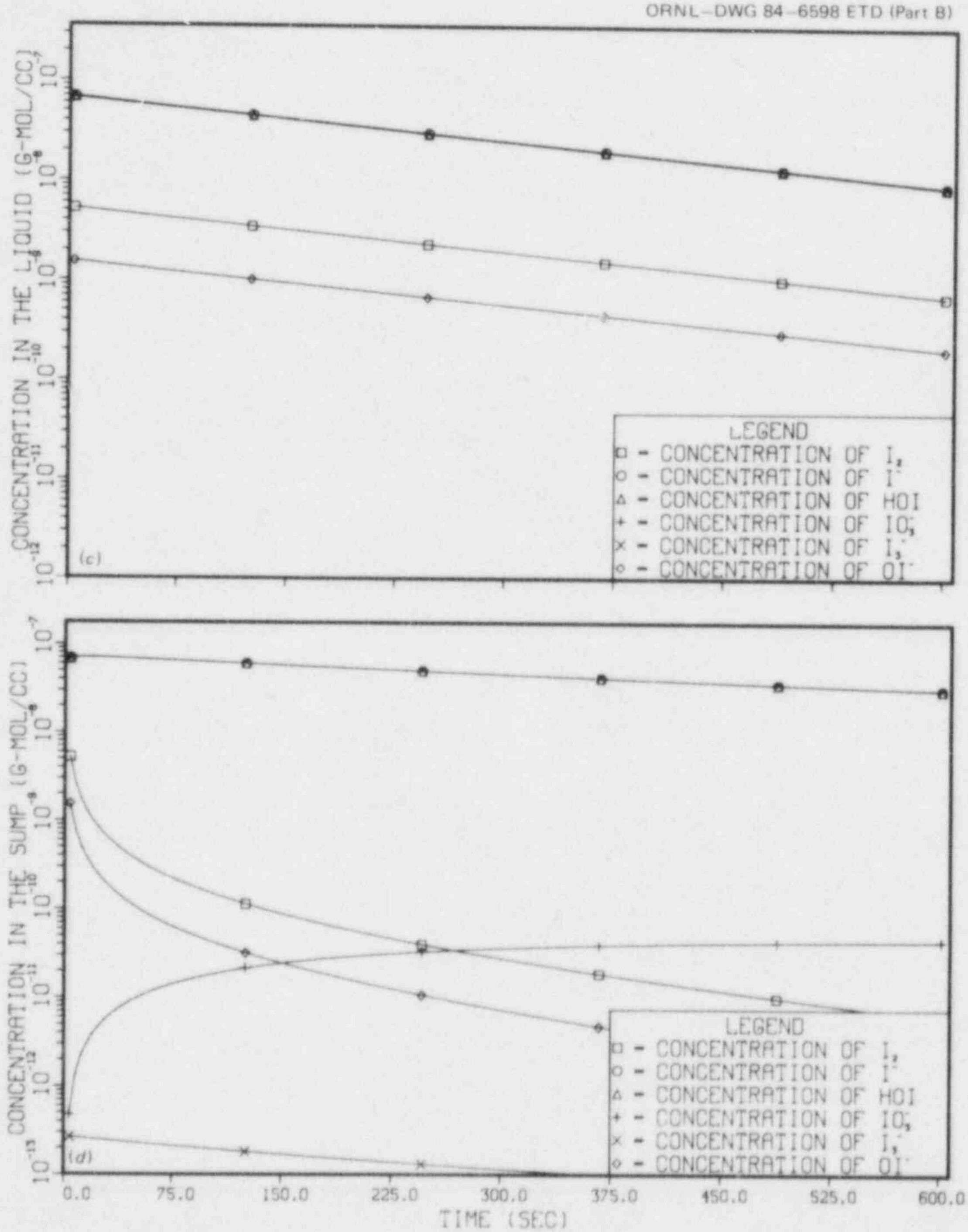


Fig. 43. (continued).

The output parameters provided by the wall spray model are the same as those calculated by the spray model. If one compares the results of the spray model to those of the wall-spray model, one will find that there is not much difference in the calculated number of moles of molecular iodine removed from the gas phase and that most of the plotted results are nearly the same. These results show that the removal of gaseous iodine by the water on the wall is approximately as important as the removal of gaseous iodine by the spray drops. But wall spray model requires much more CPU time than does the spray model and yet does not predict significantly different results from the spray model. Therefore, it is suggested that the spray model can be used in most cases for predicting the absorption of gaseous iodine by water sprays. Nevertheless, there are probably times when the results of the two models would differ significantly such as for cases in which the wall surface area is very large.

7. EXPERIMENTAL DATA

The experimental data used to compare with the results of the spray model are from the Containment System Experiments (CSE).[3] Experimental runs A-3, A-4, A-6, A-7, and A-8 of this series are large scale spray system tests to determine the effectiveness of a spray system for removing airborne fission products. The results of these tests are reported in terms of the gas phase elemental iodine concentration versus time and also in terms of the liquid phase elemental iodine concentration versus time. The parameters for the spray experiments are the spray flux, the drop size, the gas phase temperature, pressure, and humidity, and the liquid spray composition. The physical dimensions of the CSE vessel are listed in Table 3 and are shown in Figure 44. Since

Table 3. Physical conditions common to all spray experiments (Hillard[3])

Volume above deck including drywell	21,005 ft^3	595 m^3
Surface area above deck including drywell	6,140 ft^2	569 m^2
Surface area/volume	0.293 ft^{-1}	0.958 m^{-1}
Cross section area, main vessel	490 ft^2	45.5 m^2
Volume, middle room	2,089 ft^3	59 m^3
Surface area, middle room	1,363 ft^2	127 m^2
Volume, lower room	3,384 ft^3	96 m^3
Surface area, lower room	2,057 ft^2	191 m^2
Total volume of all rooms	26,477 ft^3	751 m^3
Total surface area, all rooms	9,560 ft^2	888 m^2
Drop fall height to deck	33.8 ft	10.3 m
Drop fall height to drywell bottom	50.5 ft	15.4 m
Surface coating	All interior surfaces coated with phenolic paint.[a]	
Thermal insulation	All exterior surfaces covered with 1-in. fiberglass insulation.[b]	

[a]Two coats Phenoline 302 over one coat Phenoline 300 primer. The Carboline Co., St. Louis, Missouri.

[b]k = 0.027 Btu/(hr) (ft^2) (°F/ft) at 200°F, Type PF-615, Owens-Corning Fiberglass Corp.

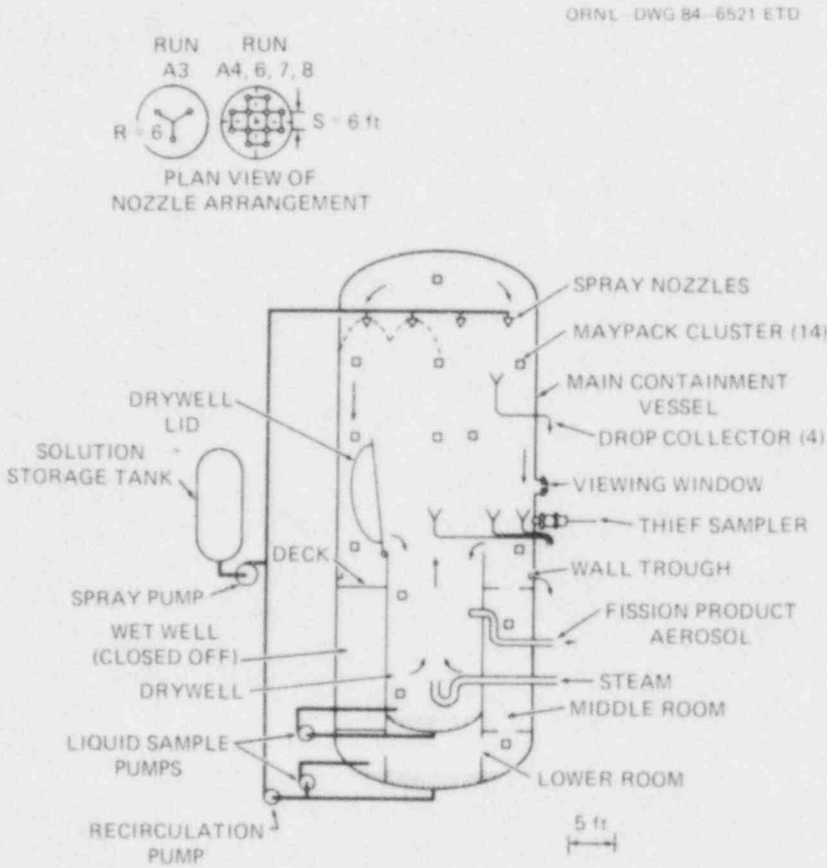


Fig. 44. Schematic diagram of containment arrangement used in CSE spray tests (Hillard[3]).

these tests were made in realistic and not idealized equipment and conditions, the liquid and gas flow patterns are complex and not well characterized. The results from the new spray model will be compared with these results, but no better than approximate agreement can be expected. This data, however, can still provide a means for useful and meaningful evaluation of the spray model.

The CSE vessel is a large scale vessel (see Table 3 and Figure 44). The overall dimensions of the vessel are 20.34 meters high and a diameter of 7.62 meters. The vessel has a drop fall height of 15.4 meters. The overall volume of the vessel is 751 cubic meters.

The tests varied the temperature, pressure, pH of the drop, spray nozzle configuration and drop size. The conditions for run A-3 are a temperature of 298K, 1 atmosphere of pressure, pH of 9.5 and a drop diameter of 1210 microns. For all of the tests, the spray solution temperature was at 25°C, and the solutions were all buffered. For run A-4, the conditions were the same as for A-3 except for a higher spray flow rate and a different spray nozzle configuration. Run A-6 increased the temperature of the gas to 397K and the pressure to 3 atmospheres. Run A-7 changed the pH to 5, lowered the temperature to 394K and raised the

pressure to 3.4 atmospheres. Run A-8 changed the drop diameter to 770 microns. See Figure 44 for spray nozzle arrangements, Table 4 for spray nozzles used, Table 5 for the atmospheric conditions, Table 6 for the spray flow rates and solutions used in the tests and Table 7 for the timing of the spray periods.

The experimental procedure for the molecular iodine spray absorption tests involved first heating the containment vessel with steam until the specified temperature was reached. A flask containing molecular iodine traced with 1 curie of iodine-131 was heated electrically. Air was passed over the flask to release molecular iodine. Samples were taken prior to turning on the sprays to determine how molecular iodine behaves without sprays. After the first spray period

Table 4. Nozzles used in CSE spray experiments (Hillard[3])

Runs A3, 4, 6, 7

Nozzle type: Spraying Systems Co. 3/4 — 7G3
Nozzle characteristics: Fog type, full cone

	A3	A4, 6, 7
Number	3	12
Layout	Triangular	Square gride
Spacing	10 ft 5 in. apart	6 ft apart
Pressure	40 psid	40 psid
Rated flow	4 gpm	4 gpm
MMD	1210 μ	1210 μ
σ_g	1.5	1.5

Run A8

Nozzle type: Spray Systems Co. 3/8 A 20
Nozzle characteristics: Fine atomization, hollow cone

Number used	12
Layout	Square grid
Spacing	6 ft apart
Pressure	40 psid
Rated flow	4 gpm
MMD	770 μ
σ_g	1.5

Table 5. Atomspheric conditions in CSE spray experiments (Hillard[3])

	Run A3	Run A4	Run A6	Run A7	Run A8
Containment vessel insulated	No	No	Yes	Yes	Yes
Forced air circulation[a]	Yes	Yes	No	No	No
Start of 1st spray					
Vapor temperature, °F[b]	77	77	255	248.7	250
Pressure, psia	14.6	14.6	44.2	50.0	50.7
Relative humidity, %	70	88	100	100	100
End of 1st spray					
Vapor temperature, °F[b]	77	77	229	234.5	243
Pressure, psia	14.6	14.6	38.6	44.4	48.2
Start of 2nd spray					
Vapor temperature, °F[b]	77	77	237	240	243
Pressure, psia	14.6	14.6	40.8	46.0	243
End of 2nd spray					
Vapor temperature, °F[b]	77	77	202	203	188
Pressure, psia	14.6	14.6	29.5	36	34.1
Start of 3rd spray					
Vapor temperature, °F[b]	77	77	233	230	218
Pressure, psia	14.6	14.6	40.7	41.8	32.2
Start of 4th spray					
Vapor temperature, °F[b]	*c*	*c*	*c*	232	247
Pressure, psia	*c*	*c*	*c*	42.4	52.4
End of 4th spray					
Vapor temperature, °F[b]	*c*	*c*	*c*	192	175
Pressure, psia	*c*	*c*	*c*	32.7	32.4

[a]Fan without duct located in bottom of drywell. 2400 ft^3/min discharge.

[b]Average of 5 thermocouples located at various elevations and radii.

[c]No fourth spray.

Table 6. Spray flow rates and solutions used in CSE experiments (Hillard[3])

	Run A3	Run A4	Run A6	Run A7	Run A8
1st spray					
Total flow rate, gpm	12.8	49	49	49	50
Volume sprayed, gal	128	490	490	490	150
Spraying pressure, psid	40	40	40	40	40
Solution	*a*	*a*	*b*	*c*	*b*
2nd spray					
Total flow rate, gpm	12.8	49	50	48.5	50
Volume sprayed, gal	385	1480	1500	1455	1850
Spraying pressure, psid	40	40	40	40	40
Solution	*a*	*a*	*b*	*c*	*b*
3rd spray					
Total flow rate, gpm	12.5	42	16	45.5	47
Volume sprayed, gal	735	1890	960	2730	2820
Spraying pressure,	40	29	4	36.5	36.5
Solution	*d*	*e*	*e*	*e*	*e*
4th spray					
Total flow rate, gpm	*g*	*g*	*g*	48.6	50.4
Volume sprayed, gal	*g*	*g*	*g*	2428	2520
Spraying pressure, psid	*g*	*g*	*g*	40	40
Solution	*g*	*g*	*g*	*f*	*f*

[a]Fresh, room temperature. 525 ppm boron as H_3BO_3 in demineralized water. NaOH added to pH of 9.5.

[b]Fresh, room temperature. 3000 ppm boron as H_3BO_3 in demineralized water. NaOH added to pH of 9.5.

[c]Fresh, room temperature. 3000 ppm boron as H_3BO_3 in demineralized water. No NaOH added. pH 5.

[d]Fresh, room temperature demineralized water.

[e]Solution in main vessel sump recirculated. No heat exchanger used.

[f]Fresh, room temperature. 1 wt% $Na_2S_2O_3$, 3000 ppm boron as H_3BO_3 in demineralized water. NaOH added to pH 9.4.

[g]No fourth spray.

Table 7. Timing of spray periods (Hillard[3])

	Time after start of iodine release, min				
	Run A3	Run A4	Run A6	Run A7	Run A8
First spray					
Start	40	40.5	30	30	30
Stop	50	50.5	40	40	33
Duration	10	10	10	10	3
Second spray					
Start	140	140	80	80	80
Stop	170	170	110	110	117
Duration	30	30	30	30	37
Third spray					
Start	1473	1205	1565	1323	200
Stop	1533	1250	1525	1383	260
Duration	60	45	60	60	60
Fourth spray					
Start	*a*	*a*	*a*	1443	1350
Stop	*a*	*a*	*a*	1493	1400
Duration	*a*	*a*	*a*	50	50

[a]No fourth spray.

of each run was started, many samples were taken from the gas phase, from the liquid in the sump, from the wall trough and from the spray drop collectors. When the first spray period was ended, more samples were taken to determine how molecular iodine acts. A second, third, and sometimes a fourth spray period were used with many samples taken from the gas and liquid phases. The gas phase concentrations were determined by Maypack samplers (see Figure 45), and the liquid phase concentrations were determined by measuring the amount of iodine-131 tracer present. For more information see Reference 3.

Results of these experimental tests are shown in Figures 46 through 55 and Table 8. Table 8 shows the material balance of iodine for all of the experimental runs. It should be noted in this table that between 25.65% and 57.58% of the iodine delivered to the containment vessel is unaccounted for and is assumed to be deposited on surfaces. Figures 46 through 50 show the concentration of elemental iodine in the gas phase as a function of time. The data is reported in terms of the half life

Table 8. Iodine material balances
(Hillard[3])

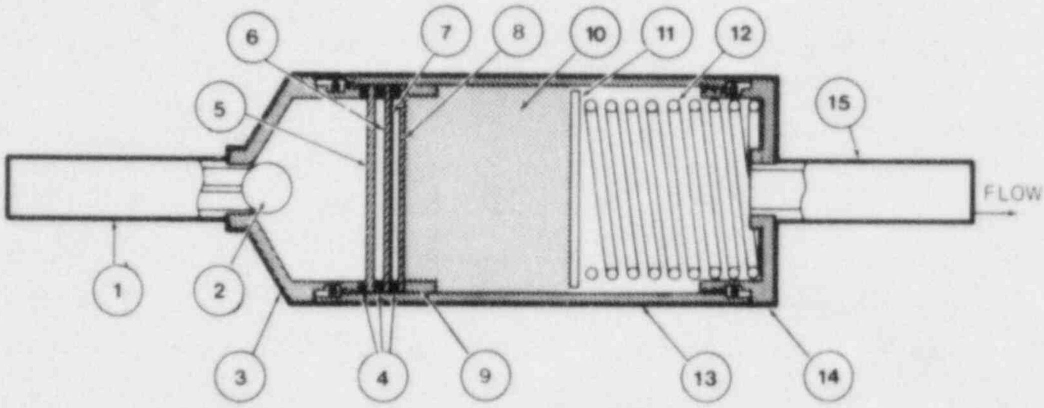
Location	Run A3		Run A4		Run A6		Run A7		Run A8	
	Grams	%[a]	Grams	%[a]	Grams	%[a]	Grams	%[a]	Grams	%[a]
					Aerosol Generation					
Starting material	101.00	100.00	101.50	100.00	101.00	100.00	101.00	100.00	101.00	100.00
Generation apparatus	2.57	3.54	1.13	1.11	0.14	0.14	1.06	1.05	3.45	3.42
Injection line	22.32	22.09	29.32	28.99	1.49	1.47	2.05	2.03	1.62	1.60
Injection line samples	0.36	0.36	0.15	0.15	1.030	1.02	0.32	0.32	0.32	0.32
Accounted for	25.25	25.00	30.59	30.14	2.66	2.63	3.43	3.40	5.39	5.34
Delivered to containment (by difference)	75.75	75.00	70.91	69.86	98.34	97.36	97.57	96.60	95.61	94.68
	Grams	%[b]	Grams	%[b]	Grams	%[b]	Grams	%[b]	Grams	%[b]
					Containment					
Delivered to containment	75.75	100.00	70.91	100.00	98.34	100.00	97.57	100.00	95.61	100.00
In liquid pools[c] (Prior to decontamination)	45.32	59.83	37.67	53.11	53.97	54.88	39.28	40.26	53.15	55.59
Samples	0.48	0.63	8.87	12.51	0.556	0.57	0.59	0.60	0.88	0.92
Purge to stack	0.52	0.69	0.73	1.03	0.086	0.09	0.16	0.17	0.11	0.11
Decontamination	5.90	7.78	5.46	7.70	0.820	0.83	1.36	1.39	1.44	1.50
Accounted for	52.22	68.93	52.73	74.35	55.43	56.37	41.39	42.42	55.57	58.12
On surfaces (by difference)	23.52	31.06	18.18	25.65	42.91	43.63	56.18	57.58	40.04	41.88

[a]Percent of starting mass.

[b]Percent of delivered mass.

[c]Includes spray solution and steam condensate.

ORNL-DWG 84-6533 ETD



1 INLET
2 TEFLON BALL
3 NOSE CONE
4 TEFTON GASKET
5 TWO PARTICLE FILTERS
6 SIX SILVER PLATED SCREENS
7 SILVER MEMBRANE FILTER
8 CHARCOAL LOADED FILTER
9 STOP RING
10 CHARCOAL BED
11 SCREEN
12 SPRING
13 BODY
14 END CAP
15 OUTLET

Fig. 45. Maypack Sampler.

of iodine, defined as

$$t_{1/2} = - \text{Ln}\ (1/2)/\lambda \ , \qquad (65)$$

$$= 0.693/\lambda \ , \qquad (66)$$

where λ is the removal rate constant.

The reason the data are in this form is because the old spray models (Equations 1 through 7 of Chapter I, Section 2) are in terms of the removal rate constant. Figures 51 to 55 shows the concentration of iodine in the liquid versus time. As can be seen in these figures, there is a delay in the response of the increase in the concentration of iodine in the liquid phase.

In these tests there are many processes for the removal of molecular iodine from the gas phase. In these large scale realistic tests, there are painted surfaces, non-painted surfaces, insulation, sprays, wet walls, and dry walls. All of these features can contribute to iodine sorption, and heat transfer can also have an effect on the removal rate of molecular iodine from the gas phase. Therefore, one can only hope to develop an approximate model which accounts for the major phenomena involved and considers only the removal by the sprays. If one looks at the drop data, these data are "difficult to interpret, not only because of sampling inadequacies but because the relative fractions of the various iodine forms and particle sizes were changing rapidly with time."[3]

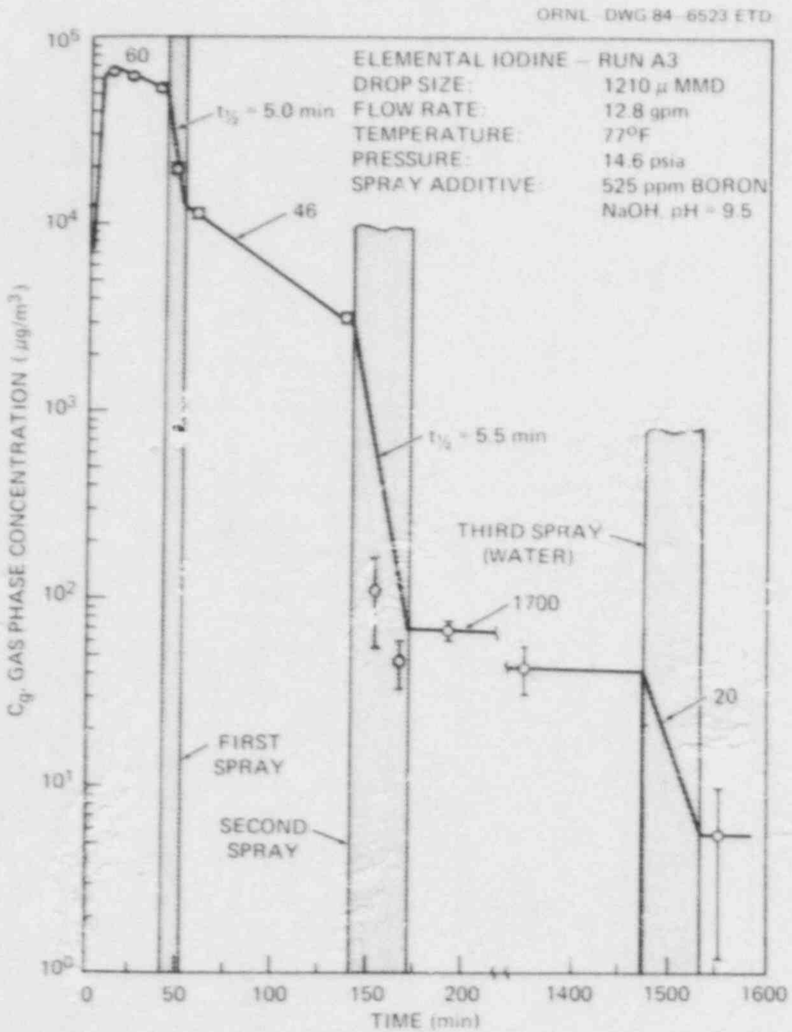


Fig. 46. Concentration of elemental iodine in the main room, run A-3 (Hillard[3]).

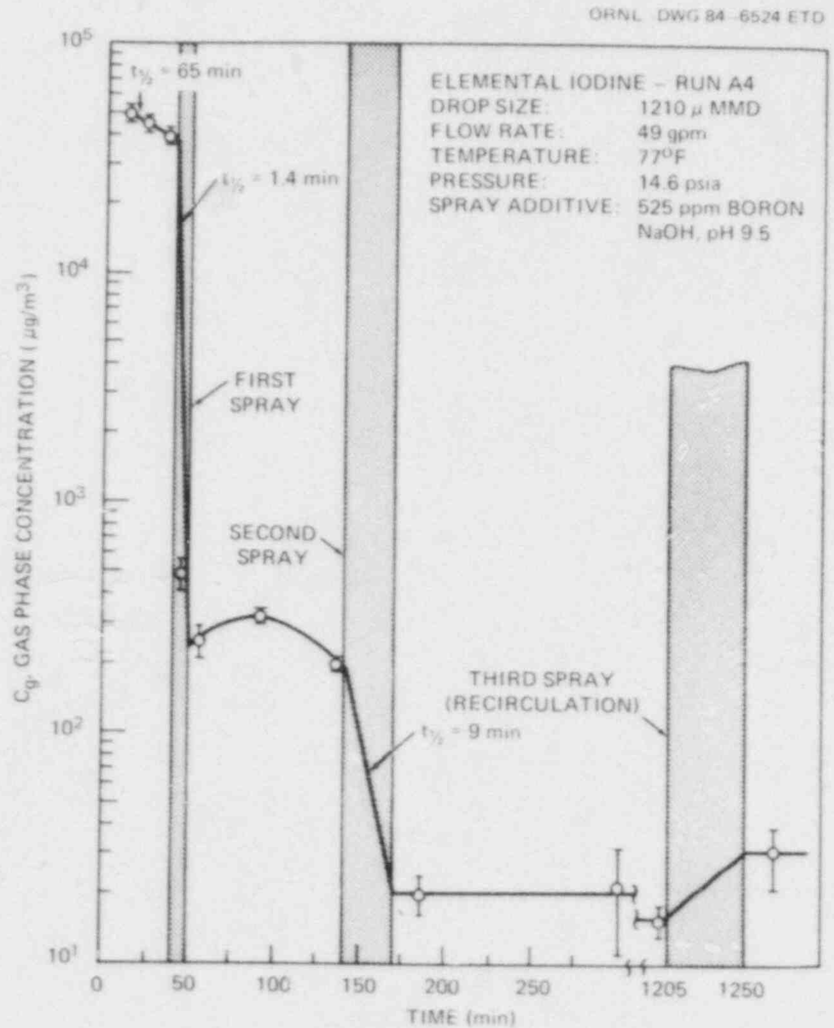


Fig. 47. Concentration of elemental iodine in the main room, run A-4 (Hillard[3]).

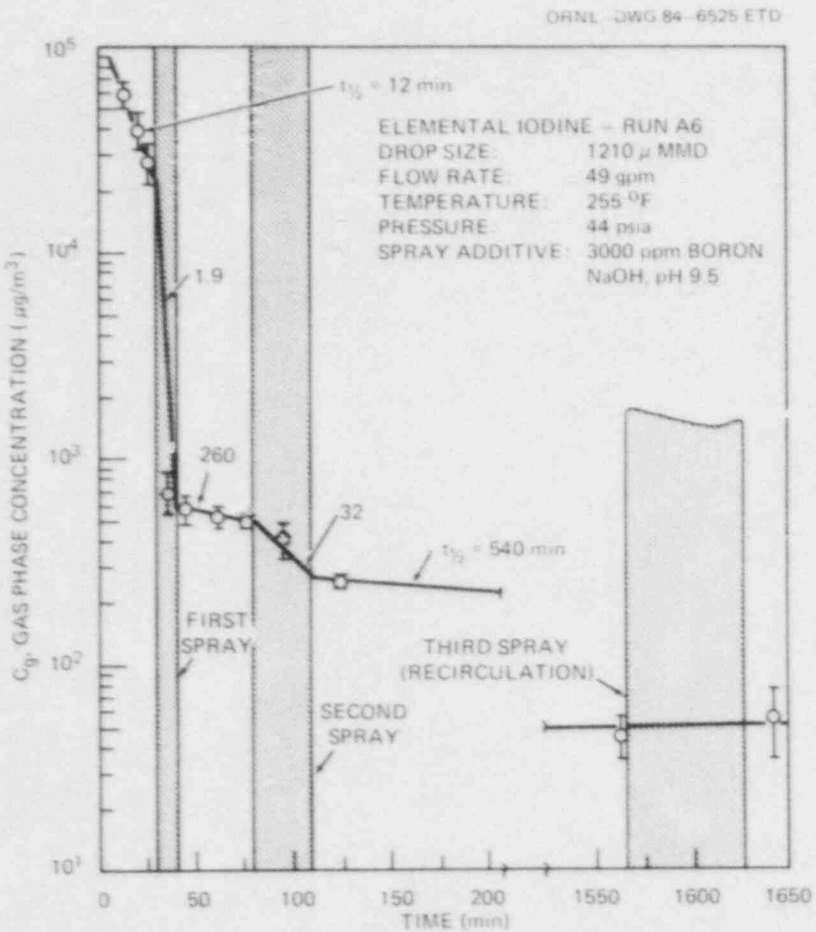


Fig. 48. Concentration of elemental iodine in the main room, run A-6 (Hillard[3]).

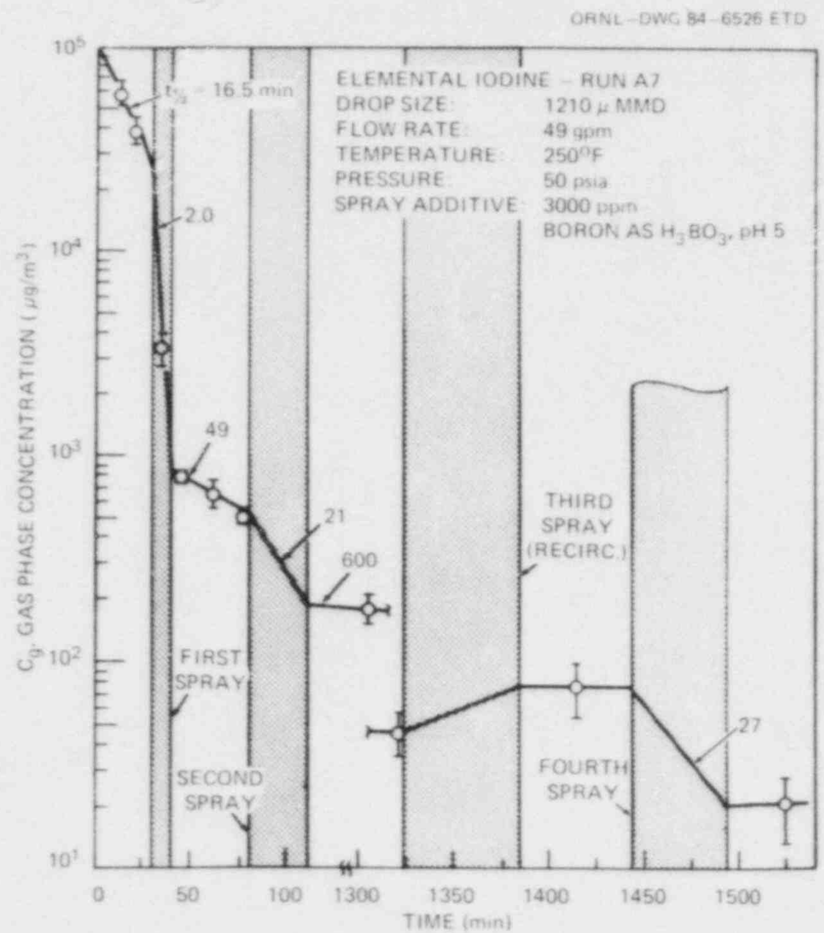


Fig. 49. Concentration of elemental iodine in the main room, run A-7 (Hillard[3]).

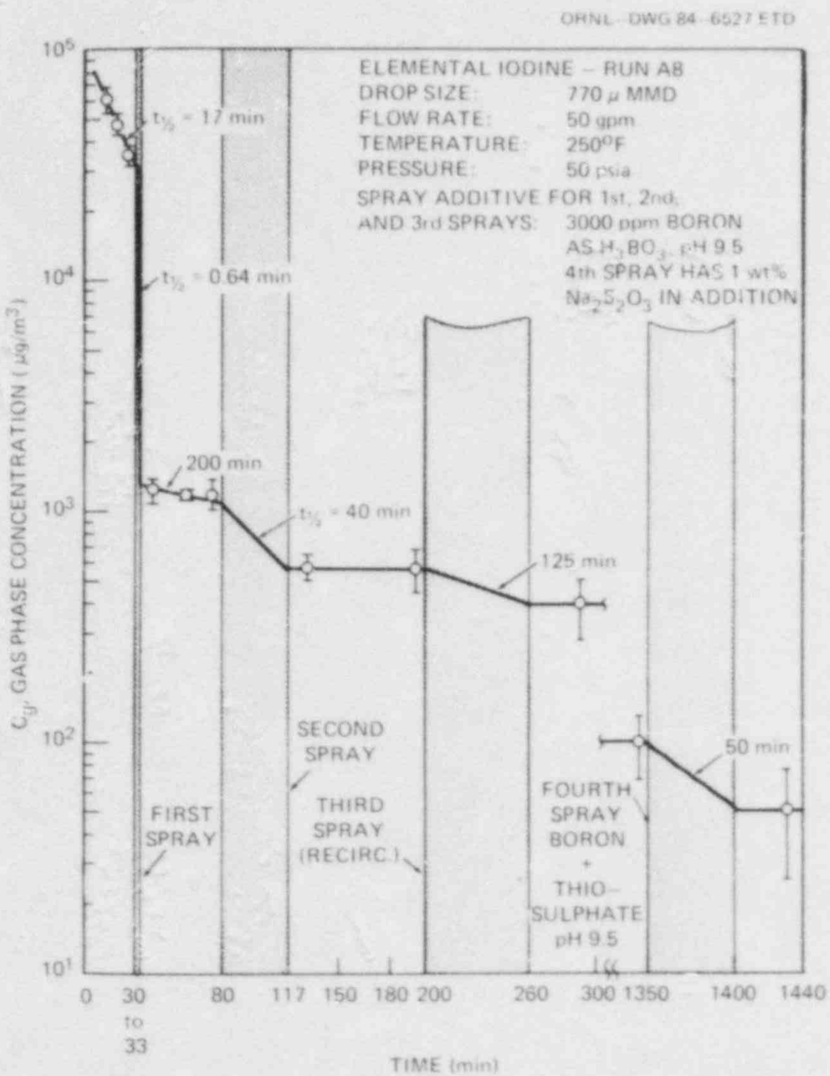


Fig. 50. Concentration of elemental iodine in the main room, run A-8 (Hillard[3]).

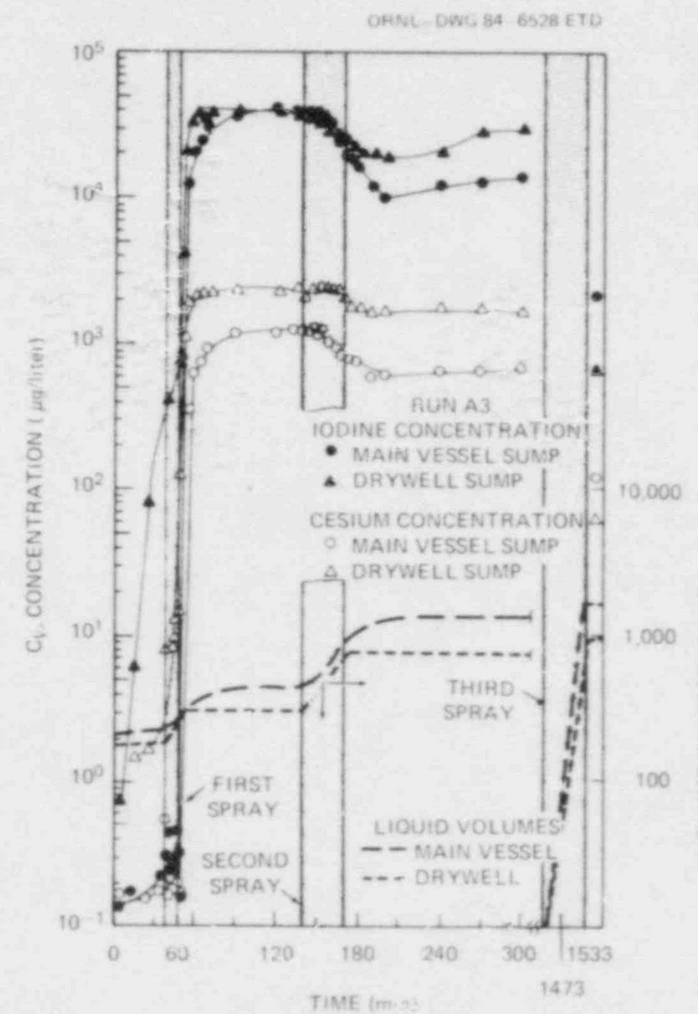


Fig. 51. Liquid volumes and concentration in vessel sumps, run A-3 (Hillard[3]).

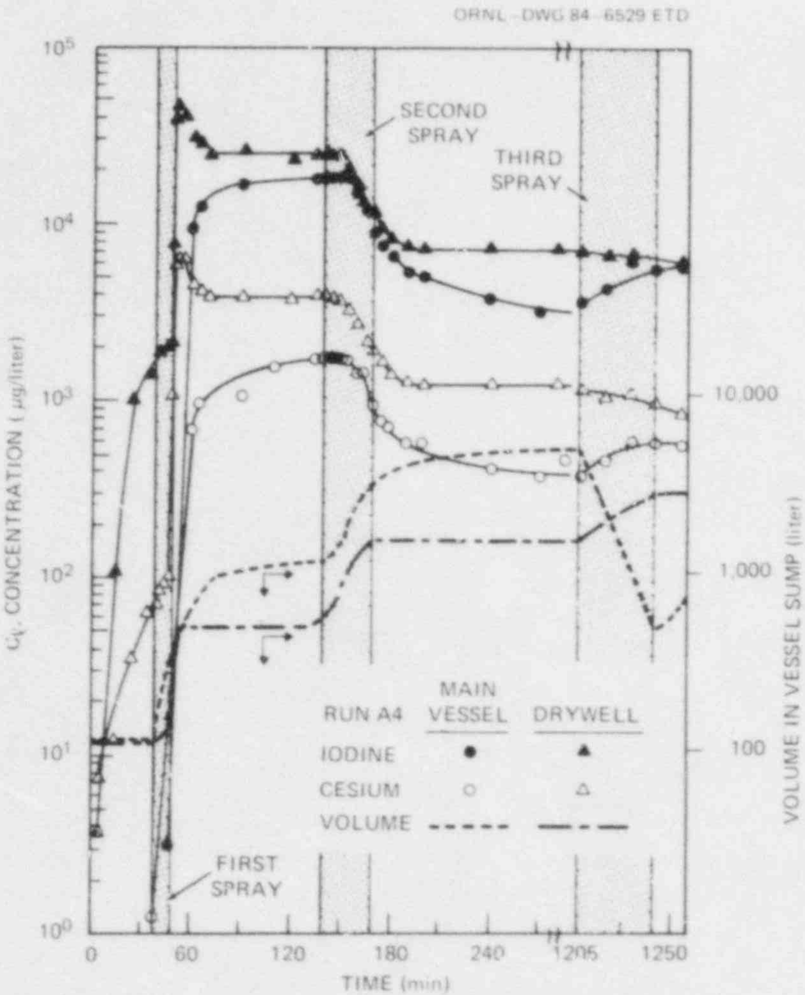


Fig. 52. Liquid volumes and concentration in vessel sumps, run A-4 (Hillard[3]).

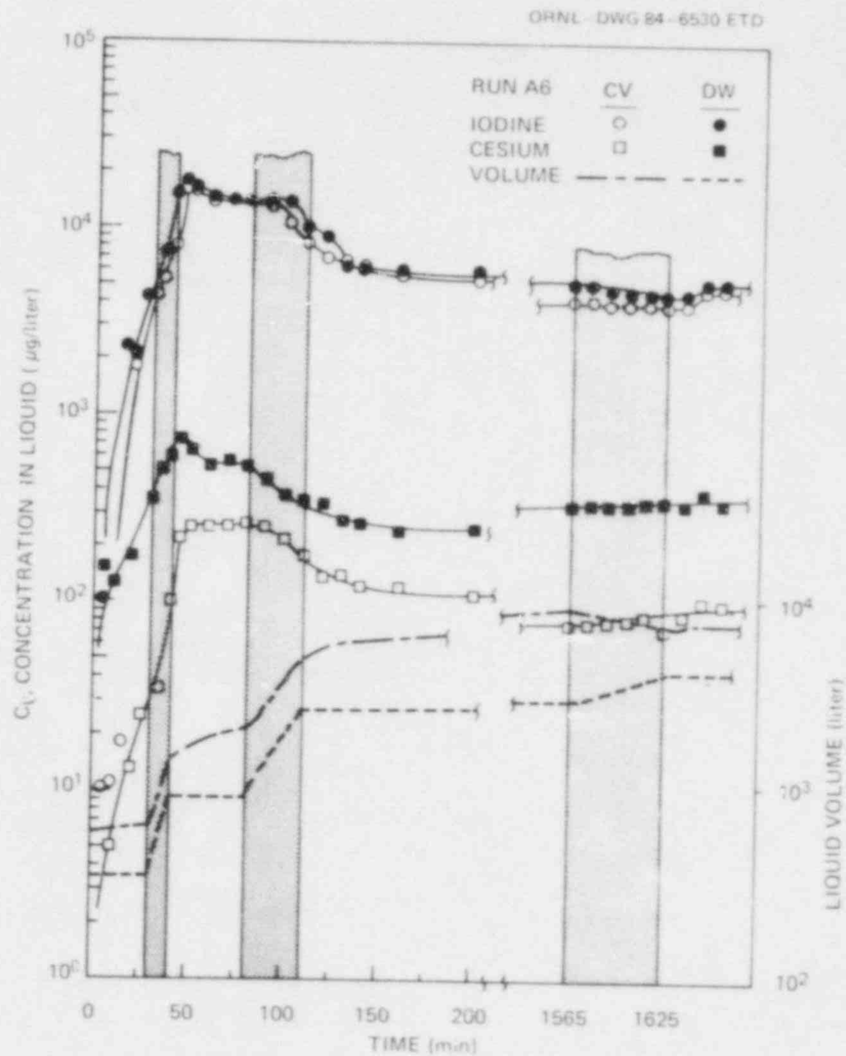


Fig. 53. Liquid volumes and concentration in vessel sumps, run A-6 (Hillard[3]).

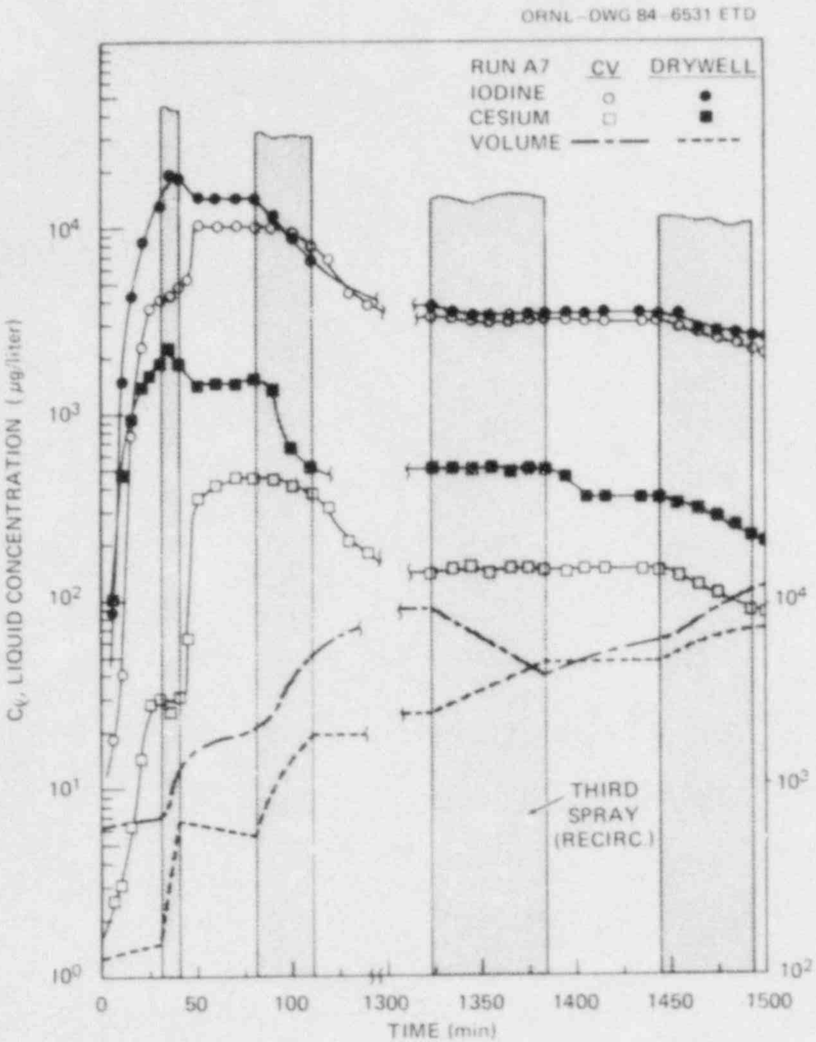


Fig. 54. Liquid volumes and concentration in vessel sumps, run A-7 (Hillard[3]).

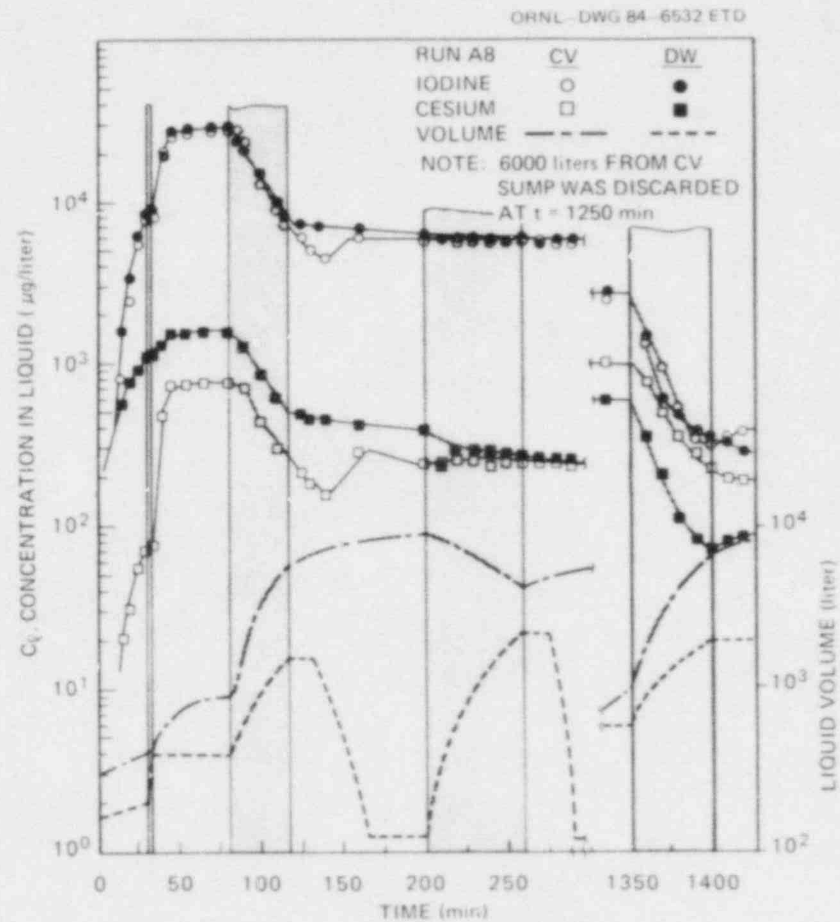


Fig. 55. Liquid volumes and concentration in vessel sumps, run A-8 (Hillard[3]).

The data for the gas phase are the result of the combined effects of all of the processes for the removal of molecular iodine from the gas phase. But if all of the processes except for the sprays exerted only a small overall effect in the removal of molecular iodine from the gas phase, then these data would be acceptable from the standpoint of usefulness in determining the efficiency of the spray model. The data for liquid in the sumps should eliminate some of the sources of error because these data shows how much molecular iodine is transferred to the liquid. Nevertheless, any iodine that is on the surfaces and is not chemically held to the walls could be washed off in the sumps. Since the sprays were not started at the instant the molecular iodine was released, a significant amount of molecular iodine released into the containment may have deposited on the surfaces, and subsequently been washed off into the sumps or might have been transferred back into the gas phase later when the partial pressure of molecular iodine in the gas phase was smaller than the partial pressure of molecular iodine on the surfaces. The latter effect could result in an underestimate of the removal rate of molecular iodine.

To remove some of the possible sources of error, the comparison of experimental results to the results of the spray model will be limited to the area of the drywell. The drywell had a cross sectional area of 8.8 square meters (which is a diameter of 3.35 meters), a drop fall height of 15.4 meters, and a volume of 135.52 cubic meters. For example, in run A-3, at the start of the first spray period, the initial gas phase concentration was approximately 5×10^4 micrograms/cubic meter (1.97×10^{-7} moles/liter) and the final concentration was approximately 1.25×10^4 micrograms/cubic meter (4.92×10^{-8} moles/liter). The amount of iodine removed from the gas phase during the first spray was 5.082 grams. Also, at the start of the first spray, the concentration of the liquid in the drywell sump was approximately 8×10^2 micrograms/liter and the initial volume was approximately 150 liters. At the end of the first spray, the concentration in the drywell sump was 4×10^4 micrograms/liter and the volume was approximately 332 liters. The number of grams of iodine transferred to the liquid in the drywell sump was 13.15 grams. The difference between the number of grams of iodine removed from the gas phase and the number of grams of iodine transferred to the liquid phase was -8.1 grams. The resulting relative error based on the gas phase is

$$\text{error} = \left(\frac{\text{grams removed from gas} - \text{grams transferred to liquid}}{\text{grams removed from gas}}\right) \times 100\% \,, \tag{67}$$

$$\text{error} = \frac{(5.082 - 13.15)}{(5.082)} \times 100\% = -133.4\% \,. \tag{68}$$

Results of the other runs were similar with more iodine appearing transferred to the liquid than was removed from the gas. In fact, for many cases the error is much greater.

Some of the errors noted above may have resulted from iodine that had deposited on the walls before the sprays had started and that was subsequently washed off into the drywell sump. This explanation appears feasible, but may not be the total answer since the highest concentration of molecular iodine in the gas phase was reported to be 6.5×10^4 micrograms/cubic meter; and with a concentration at the start of the spray period of 5×10^4 micrograms/cubic meter it appears that only 2.03 grams were removed before the first spray (from gas above the drywell area). Another explanation would be that since the volume for this comparison is constrained to the volume of the drywell, there could be a transfer of additional iodine that was previously on the surfaces back to the gas. Most likely, however, much of the error is simply due to error sampling and analytical measurements in both phases.

8. COMPARISON TO DATA AND OLD MODELS

The spray model has been compared to the large scale tests from the Containment Systems Experiments,[3] see Figures 56 through 65. The basis for the comparison is the number of grams of molecular iodine removed from the gas phase in the experimental test as opposed to the number of grams of molecular iodine that is predicted to be removed by the spray model. Since there is such a large discrepancy in the data between the gas and liquid phases (see Chapter 7, Experimental Data), only the experimental data from the drywell will be considered in an effort to eliminate some of the possible sources of error (see Table 9 for spray distributions). For run A-3 of the CSE tests, the initial conditions at the beginning of the first spray are:

Temperature of the liquid spray solution = 77°F = 298K,
Temperature of the gas = 77°F = 298K,
Pressure = 1 atmosphere,
Drop size = 1210 microns mass medium diameter,
(assumed) = 1210 microns average surface area diameter,
= 1210 microns average volume diameter,
Spray solution = buffered pH of 9.5 and all other liquid species have a concentration of 0.0 moles/liter,

Table 9. Measured spray liquid distribution in CSE tests (Hillard[3])

	Total spray volume recovered, %			
	Wall trough	Main sump	Dry well sump	Deck distribution $\pm 1\sigma$ (%)
Cross section				
Area, %	2.0	78.5	19.5	
Run A3[a]	0.7	62.8	37.5	64.8
Run A4[a]	10.9	68.9	20.2	46.7
Run A6 and A7[b]	2.1	68.4	28.5	
Run A8[a]	~6.0	73.0	21.0	46.2

[a]Measured during shakedown test.

[b]Measured from liquid level change during run. Normal condensation deducted.

ORNL-DWG 84-6579 ETD (Part A)

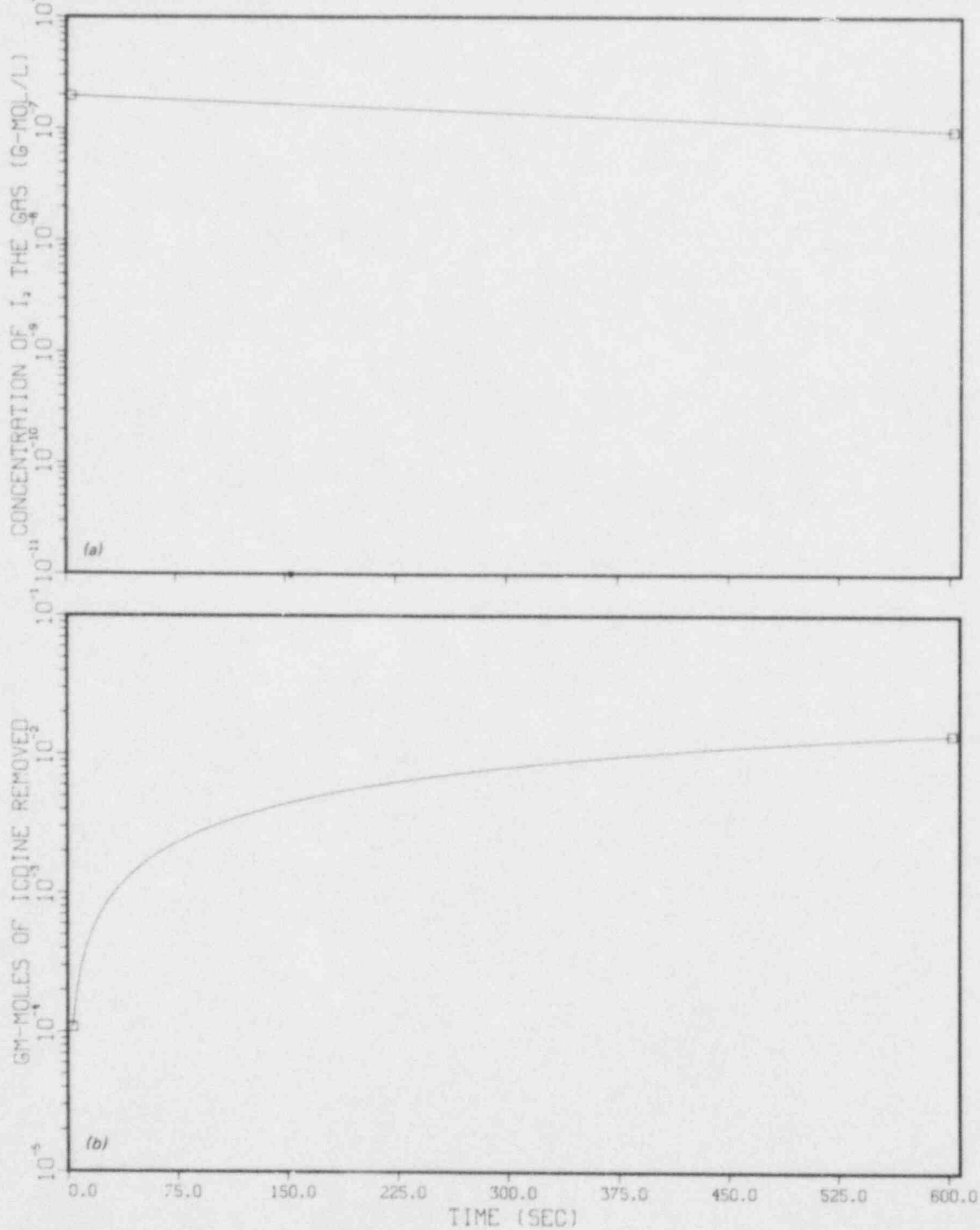


Fig. 56. Results of Spray Model for CSE run A-3 first spray period. Initial concentration of molecular iodine in the gas phase of 1.97×10^{-7} moles/liter and a buffered pH of 9.5 in the spray solution.

(a) Concentration of molecular iodine in the gas phase as a function of time.

(b) Number of moles of molecular iodine transferred as a function of time.

(c) Concentration of iodine species in the liquid drops as a function of time.

(d) Concentrati~n of iodine species in the sump as a function of time.

ORNL-DWG 84-6579 ETD (Part B)

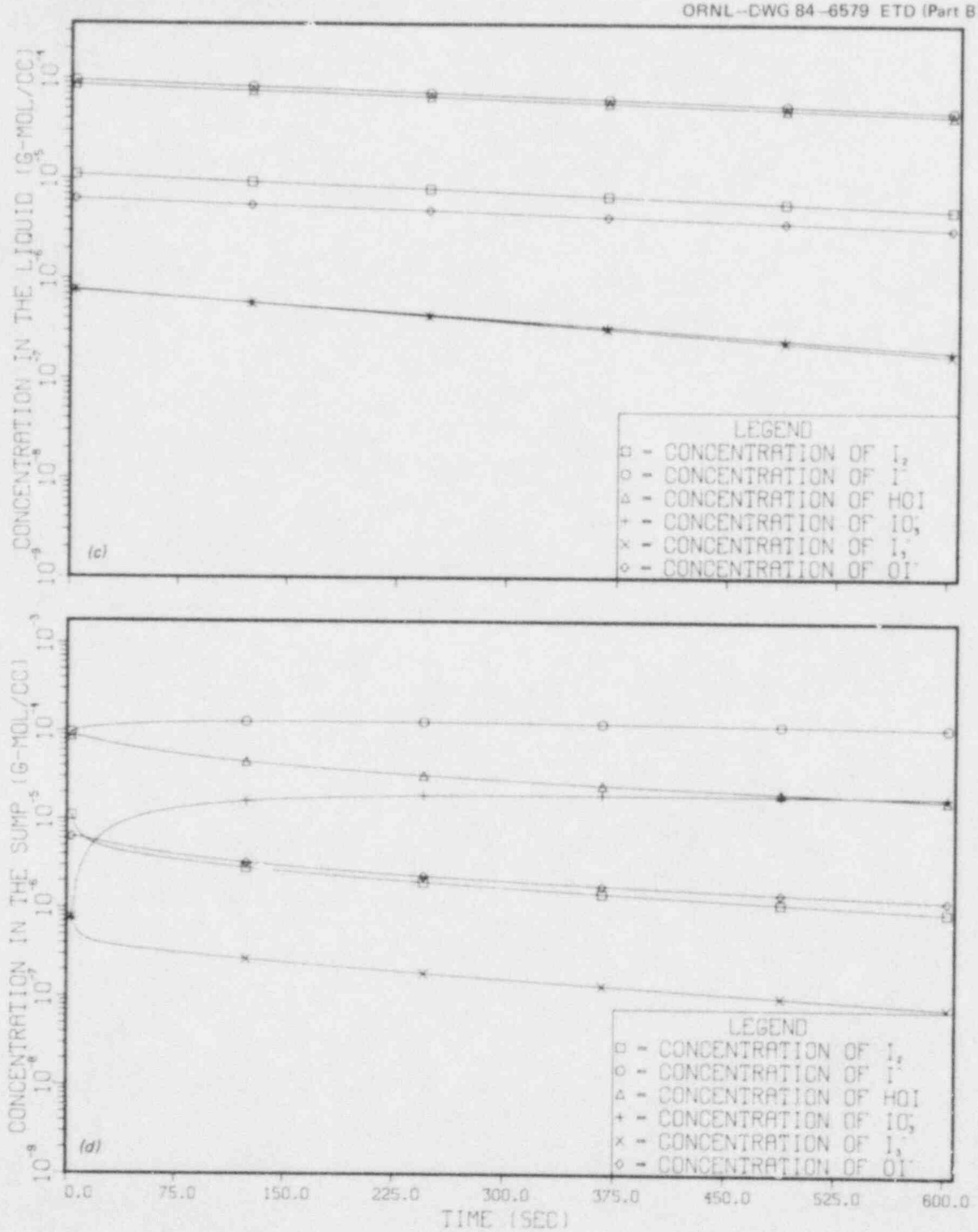


Fig. 56. (continued).

ORNL—DWG 84-6580 ETD (Part A)

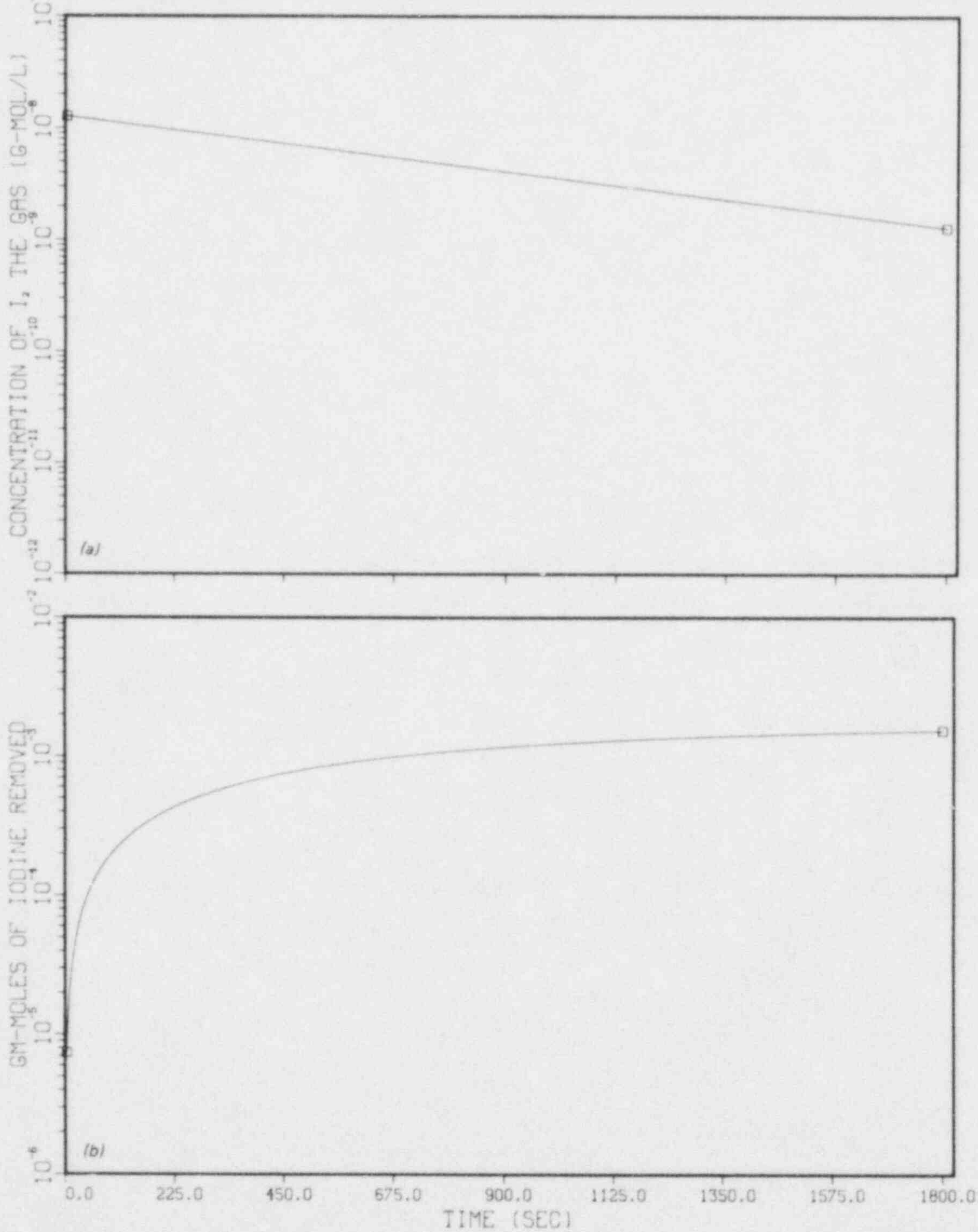


Fig. 57. Results of Spray Model for CSE run A-3 second spray period. Initial concentration of molecular iodine in the gas phase of 1.29×10^{-8} moles/liter and a buffered pH of 9.5 in the spray solution.

(a) Concentration of molecular iodine in the gas phase as a function of time.

(b) Number of moles of molecular iodine transferred as a function of time.

(c) Concentration of iodine species in the liquid drops as a function of time.

(d) Concentration of iodine species in the sump as a function of time.

ORNL-DWG 84-6580 ETD (Part B)

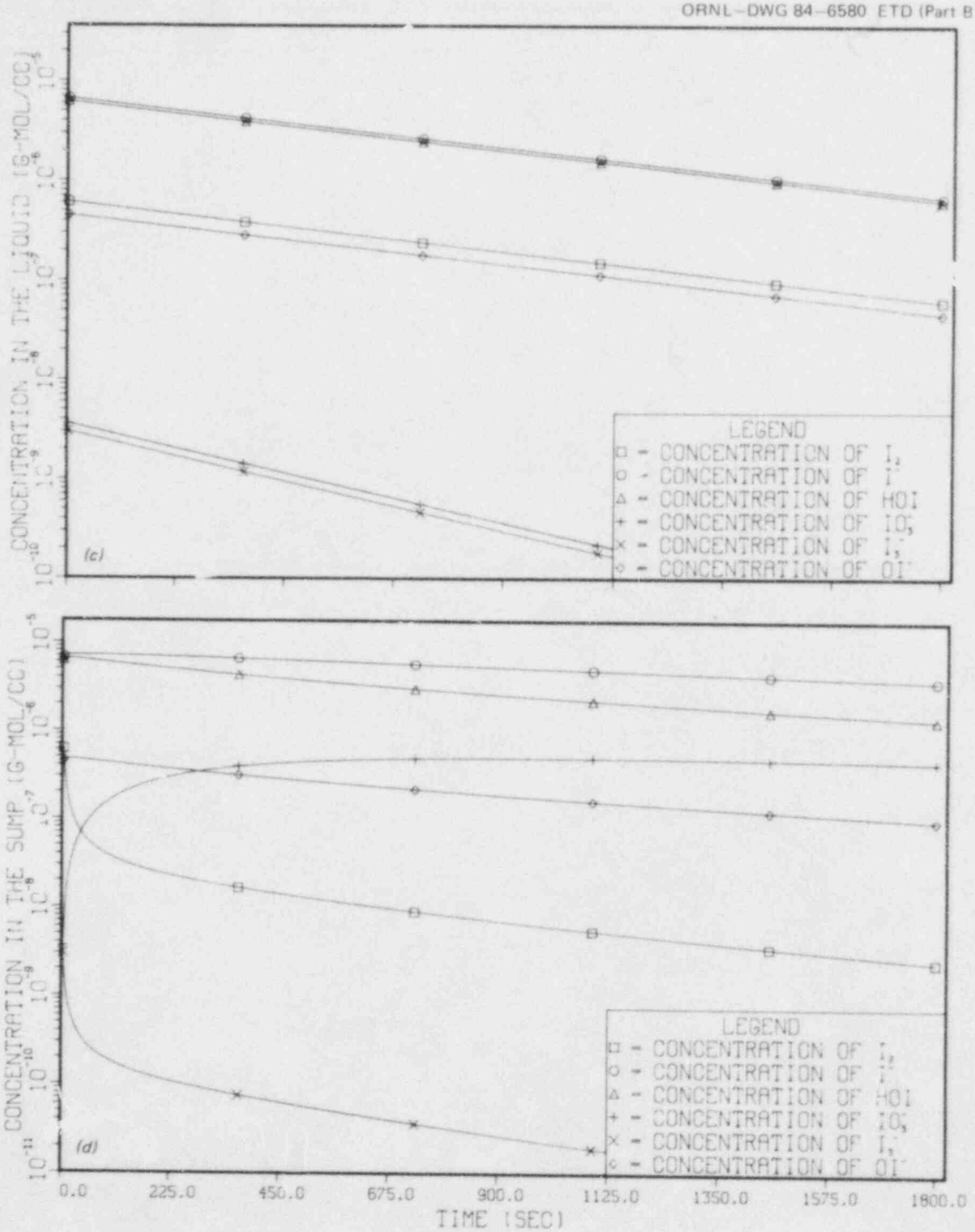


Fig. 57. (continued).

ORNL-DWG 84-6581 ETD (Part A)

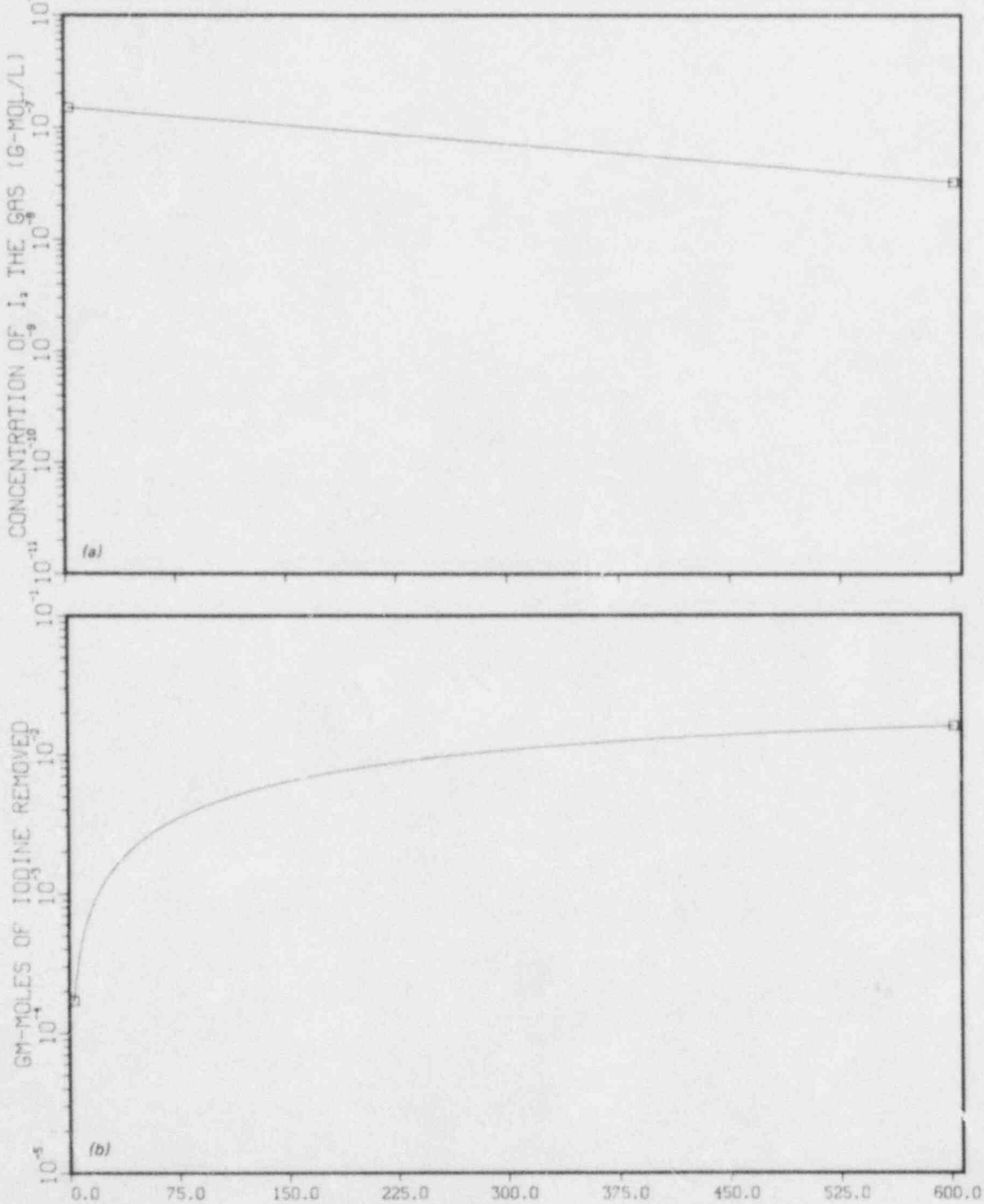


Fig. 58. Results of Spray Model for CSE run A-4 first spray period. Initial concentration of molecular iodine in the gas phase of 1.50×10^{-7} moles/liter and a buffered pH of 9.5 in the spray solution.

(a) Concentration of molecular iodine in the gas phase as a function of time.

(b) Number of moles of molecular iodine transferred as a function of time.

(c) Concentration of iodine species in the liquid drops as a function of time.

(d) Concentration of iodine species in the sump as a function of time.

ORNL-DWG 84-6581 ETD (Part B)

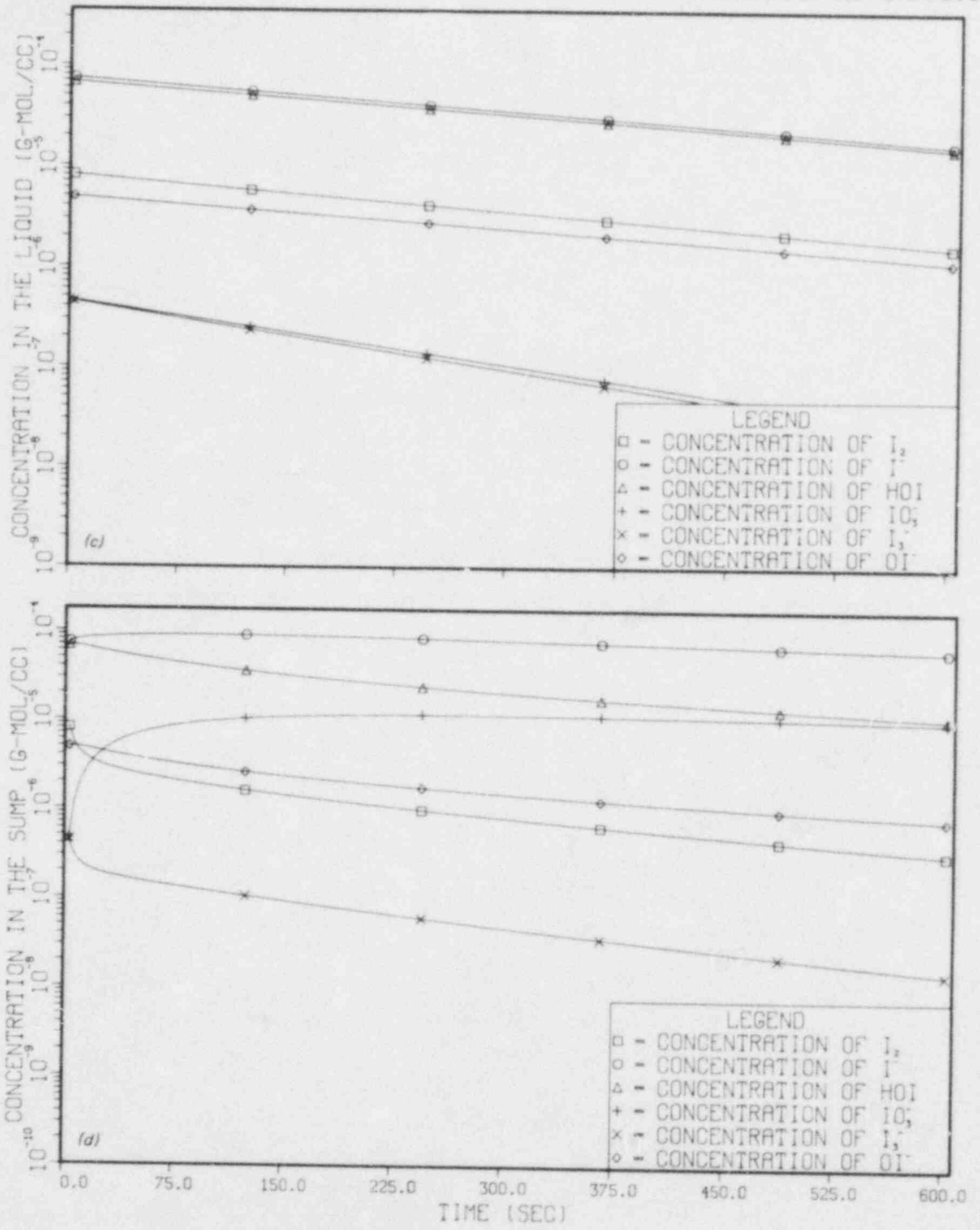


Fig. 58. (continued).

ORNL–DWG 84–6582 ETD (Part A)

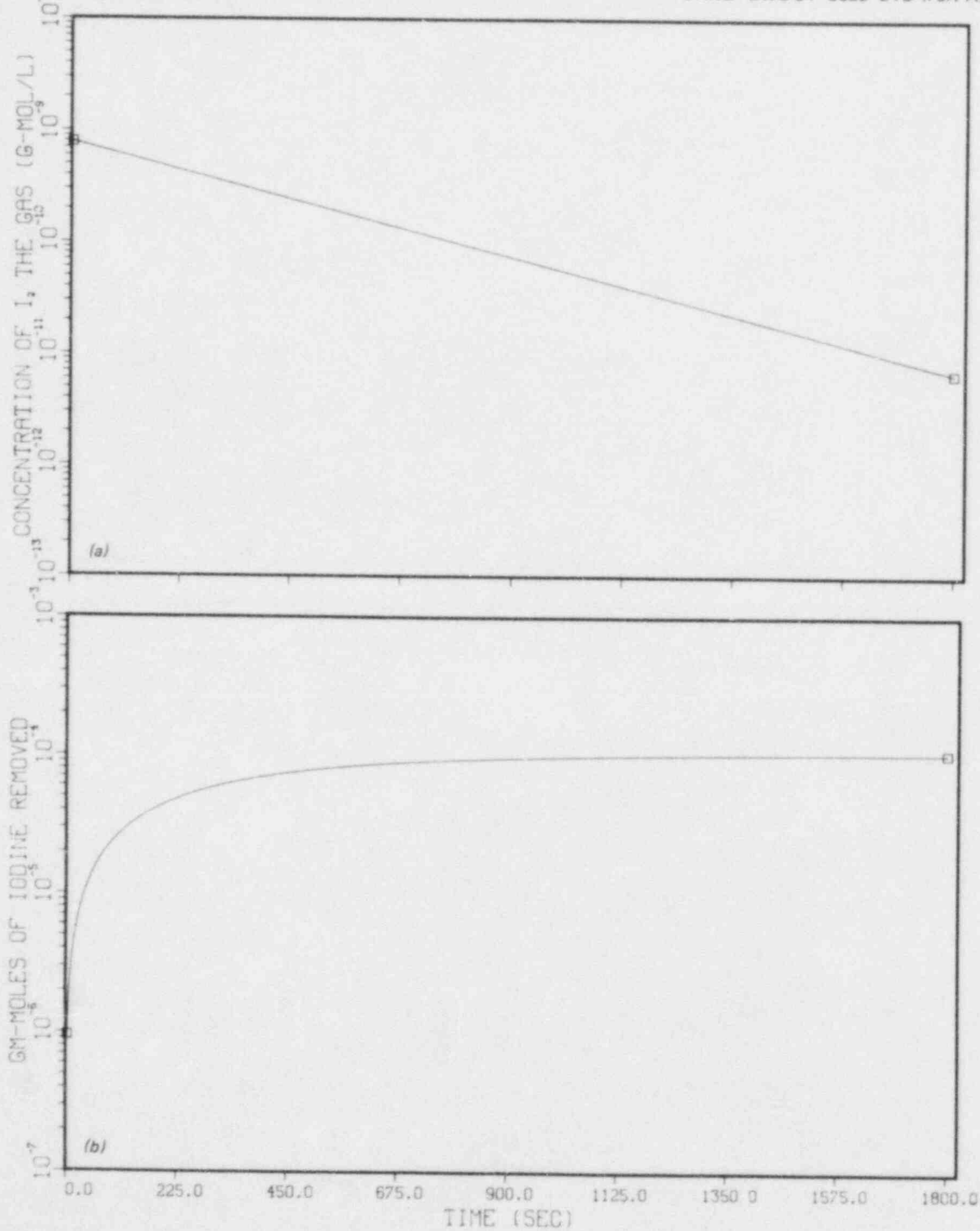


Fig. 59. Results of Spray Model for CSE run A-4 second spray period. Initial concentration of molecular iodine in the gas phase of 7.88×10^{-10} moles/liter and a buffered pH of 9.5 in the spray solution.

(a) Concentration of molecular iodine in the gas phase as a function of time.

(b) Number of moles of molecular iodine transferred as a function of time.

(c) Concentration of iodine species in the liquid drops as a function of time.

(d) Concentration of iodine species in the sump as a function of time.

ORNL-DWG 84-6582 ETD (Part B)

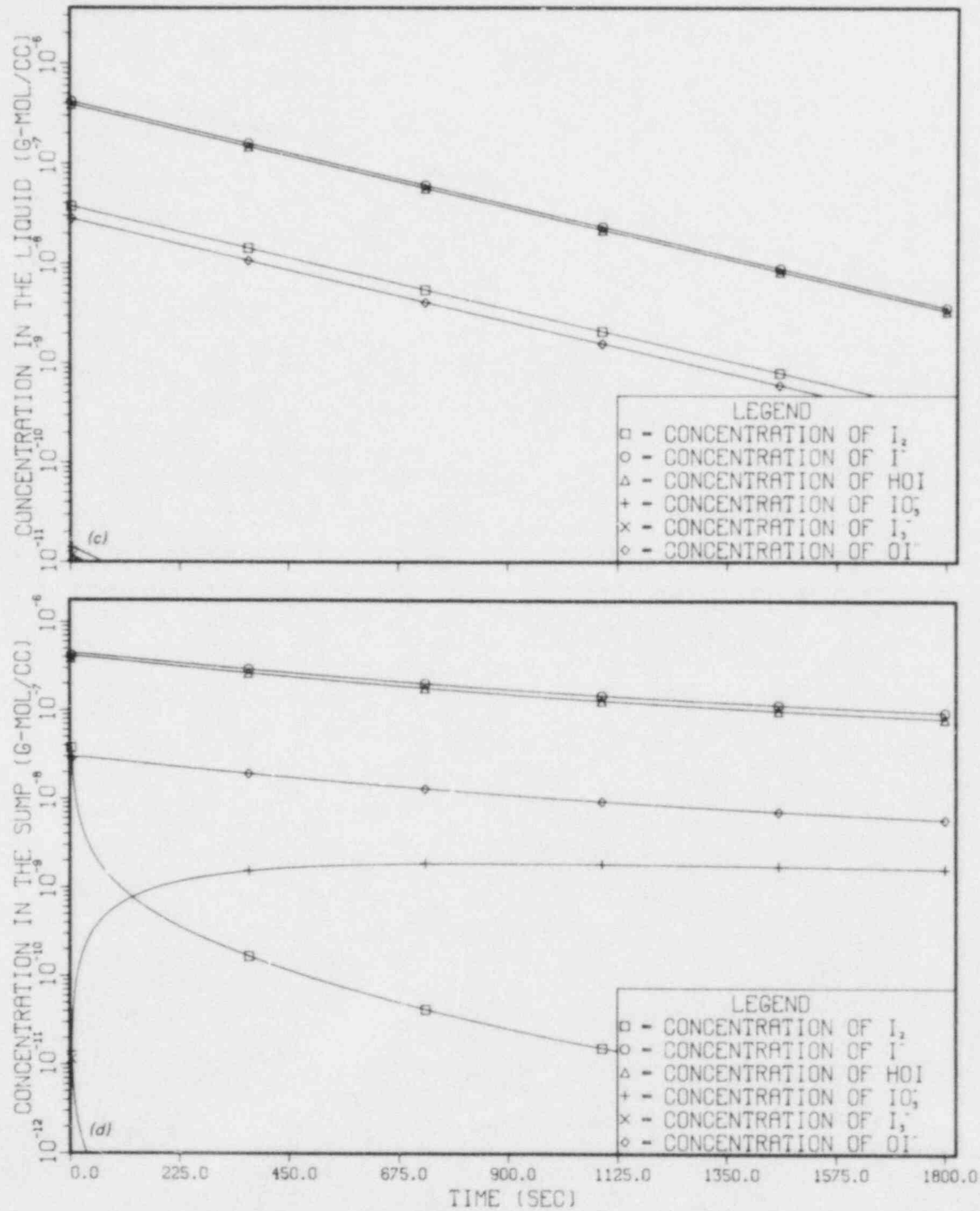


Fig. 59. (continued).

ORNL–DWG 84–6575 ETD (Part A)

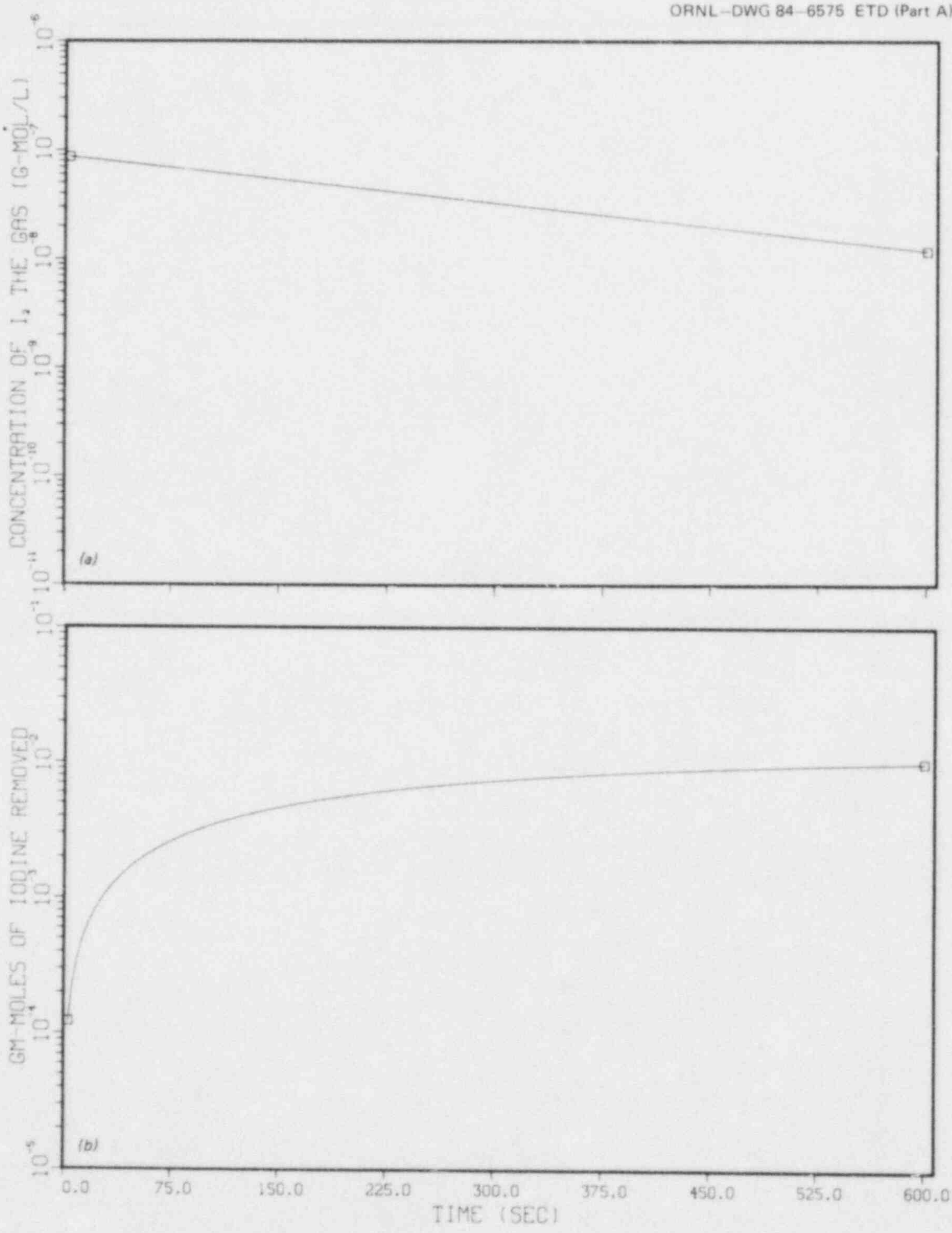


Fig. 60. Results of Spray Model for CSE run A-6 first spray period. Initial concentration of molecular iodine in the gas phase of 8.67×10^{-8} moles/liter and a buffered pH of 9.5 in the spray solution.

(a) Concentration of molecular iodine in the gas phase as a function of time.

(b) Number of moles of molecular iodine transferred as a fu ' ion of time.

(c) Concentration of iodine species in the liquid drops as a function of time.

(d) Concentration of iodine species in the sump as a function of time.

ORNL-DWG 84-6575 ETD (Part B)

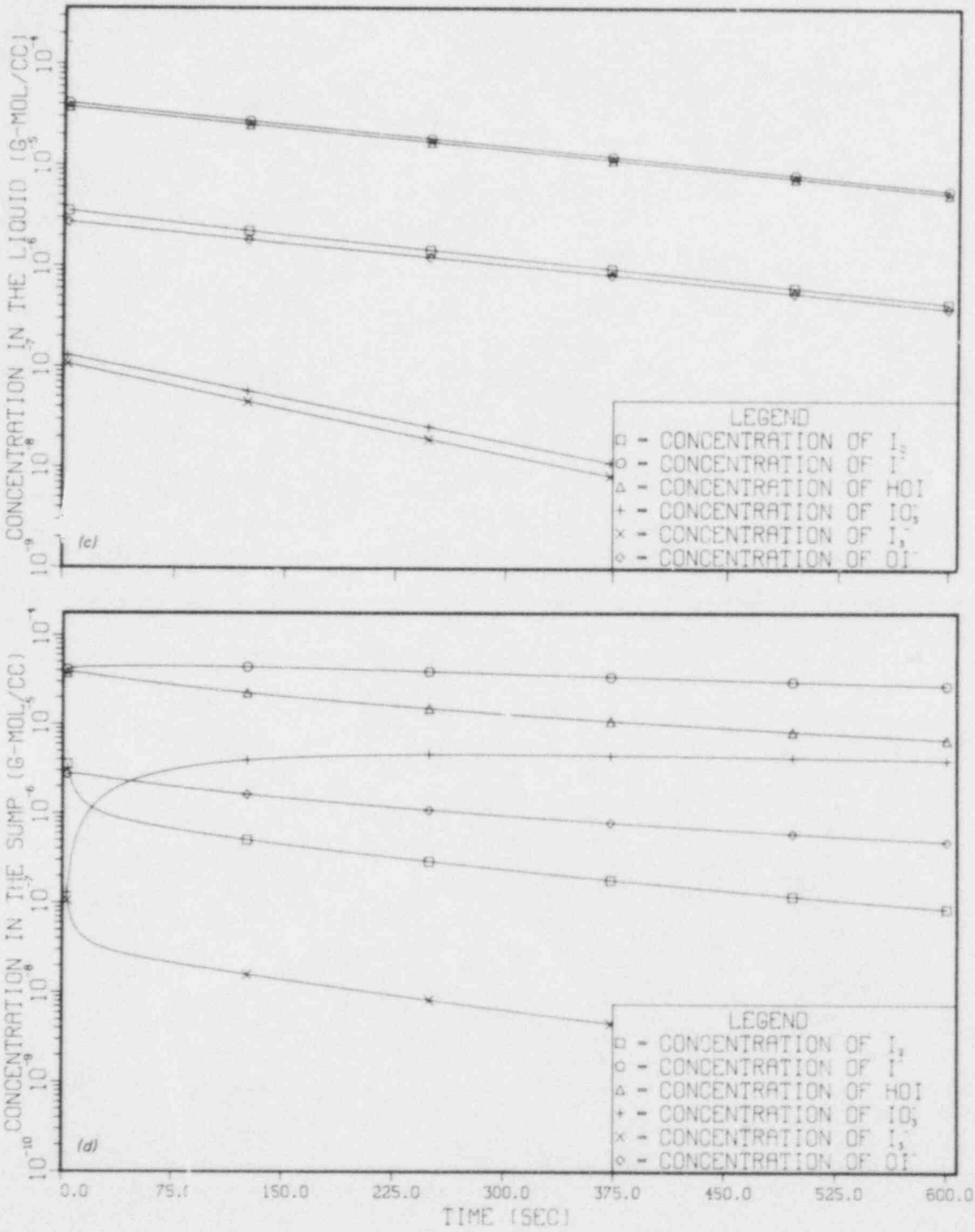


Fig. 60. (continued).

ORNL–DWG 84–6576 ETD (Part A)

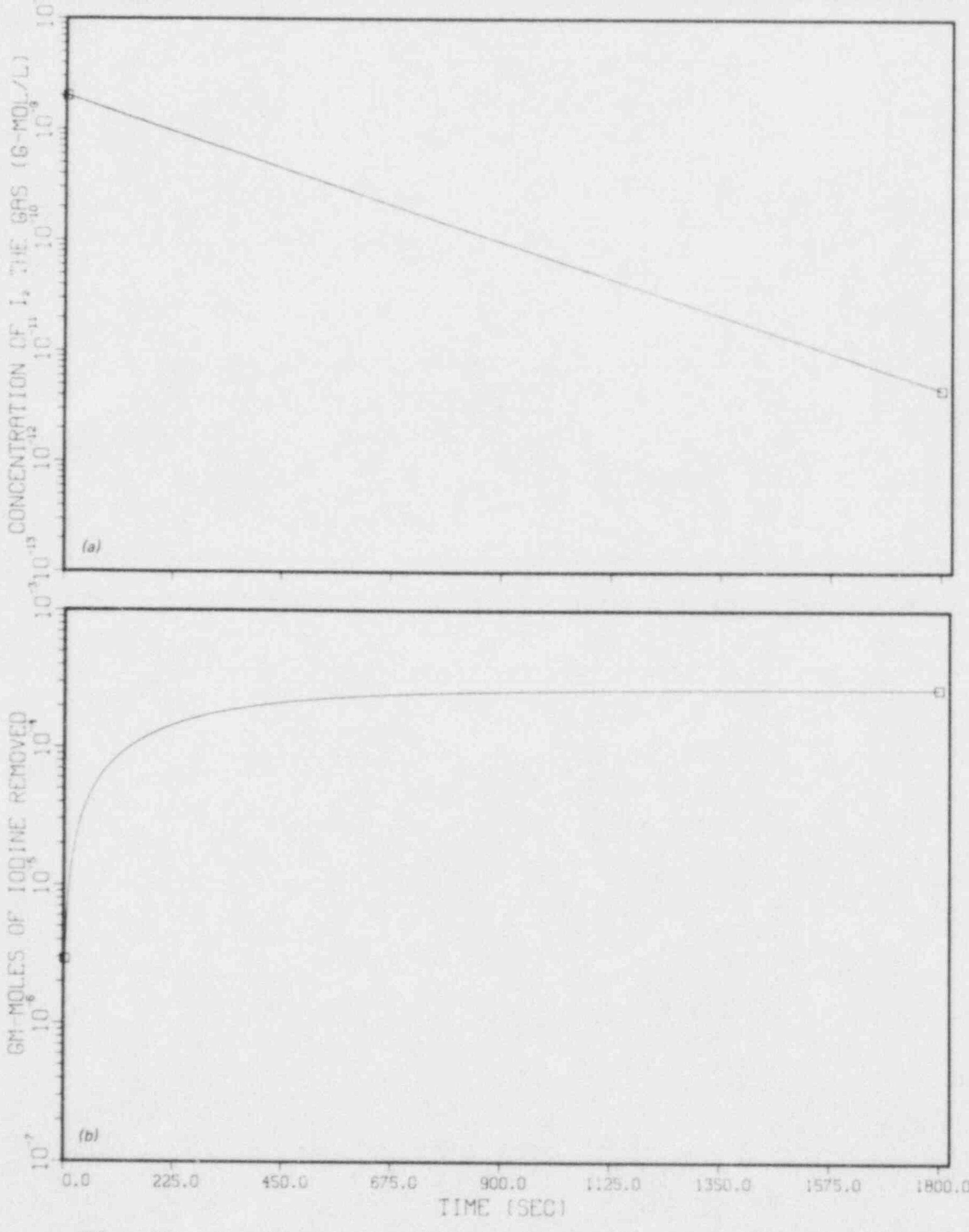


Fig. 61. Results of Spray Model for CSE run A-6 second spray period. Initial concentration of molecular iodine in the gas phase of 2.01×10^{-9} moles/liter and a buffered pH of 9.5 in the spray solution.

(a) Concentration of molecular iodine in the gas phase as a function of time.

(b) Number of moles of molecular iodine transferred as a function of time.

(c) Concentration of iodine species in the liquid drops as a function of time.

(d) Concentration of iodine species in the sump as a function of time.

ORNL–DWG 84–6576 ETD (Part B)

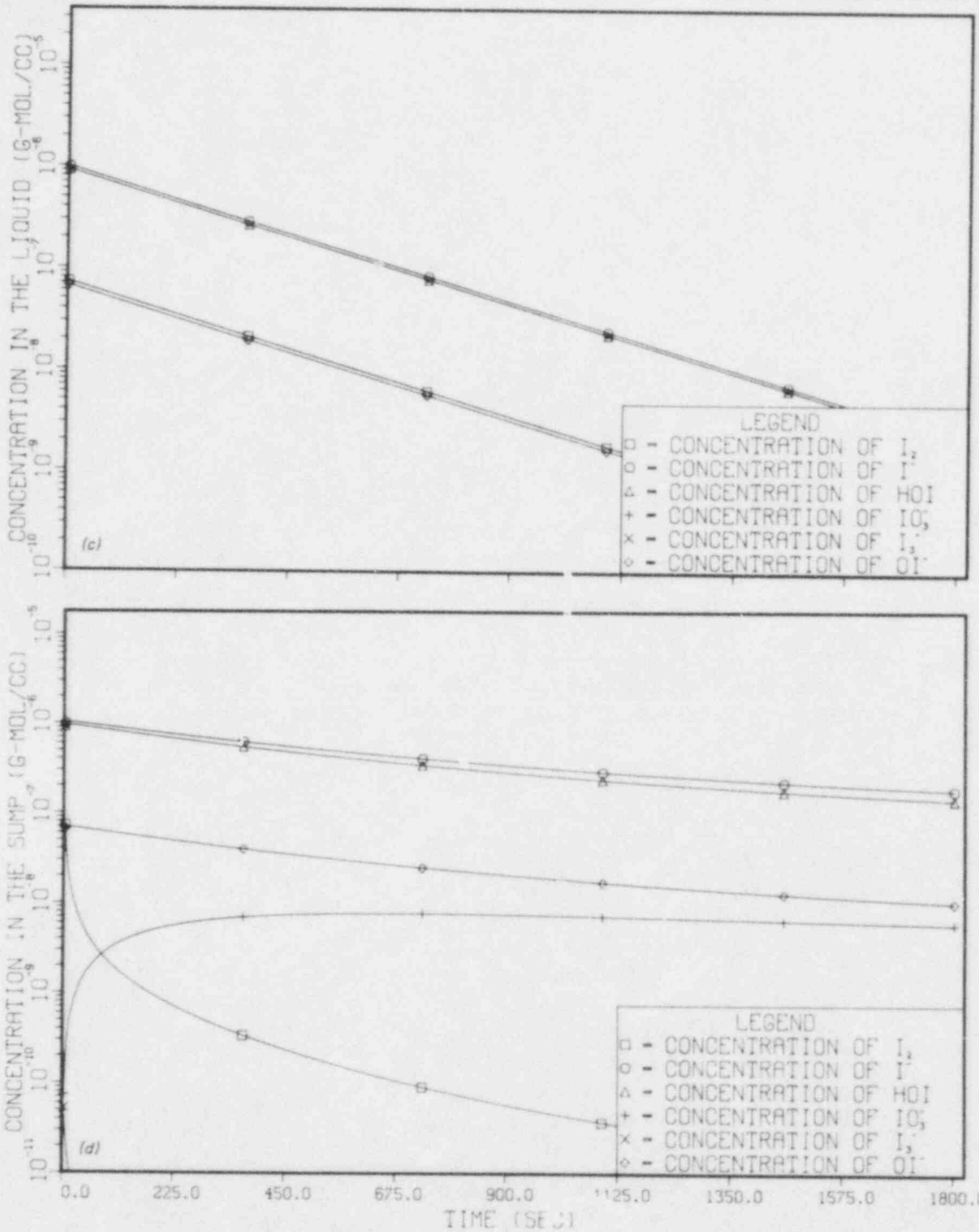


Fig. 61. (continued).

ORNL-DWG 84-6577 ETD (Part A)

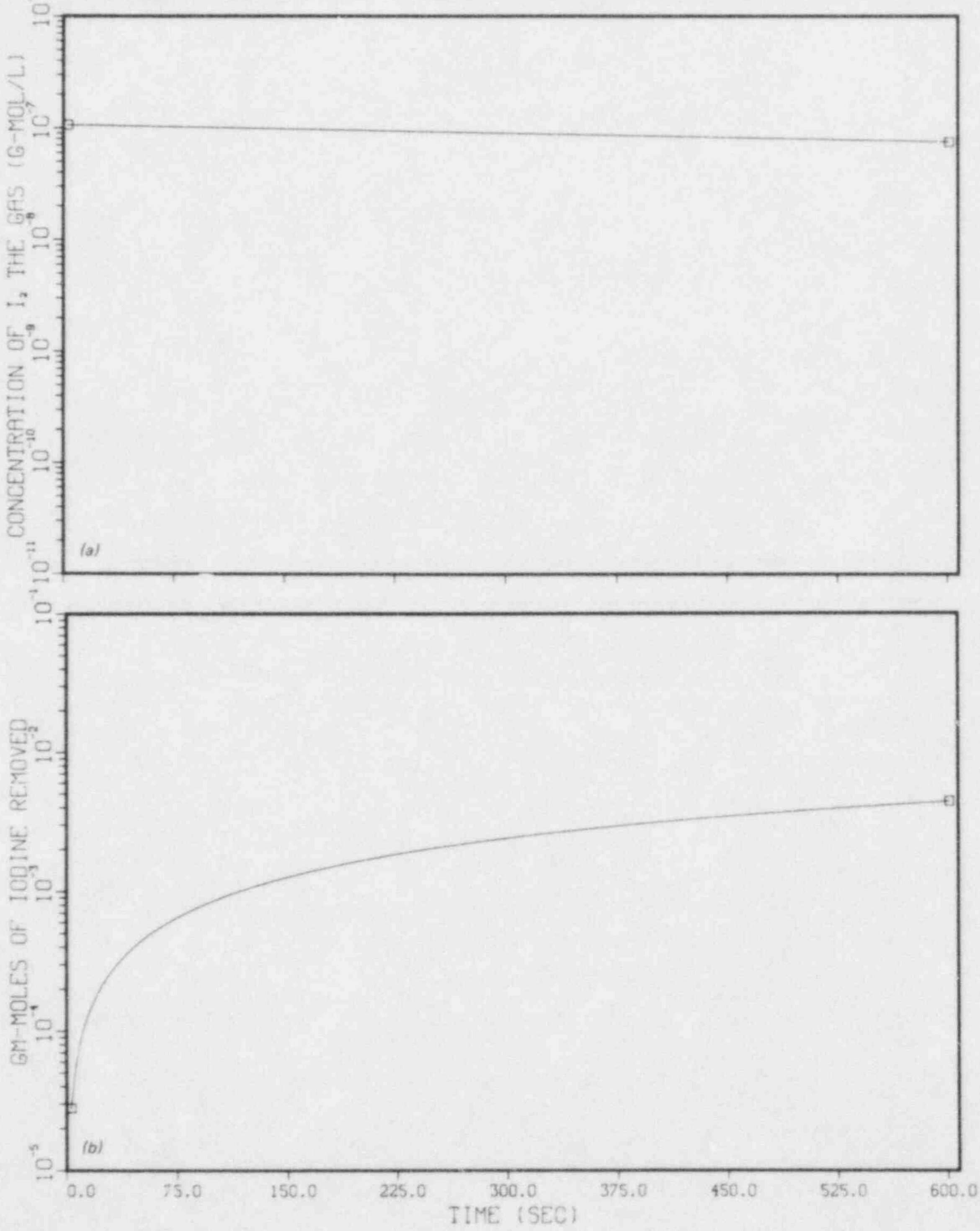


Fig. 62. Results of Spray Model for CSE run A-7 first spray period. Initial concentration of molecular iodine in the gas phase of 1.06×10^{-7} moles/liter and a buffered pH of 5.0 in the spray solution.

(a) Concentration of molecular iodine in the gas phase as a function of time.

(b) Number of moles of molecular iodine transferred as a function of time.

(c) Concentration of iodine species in the liquid drops as a function of time.

(d) Concentration of iodine species in the sump as a function of time.

ORNL-DWG 84-6577 ETD (Part B)

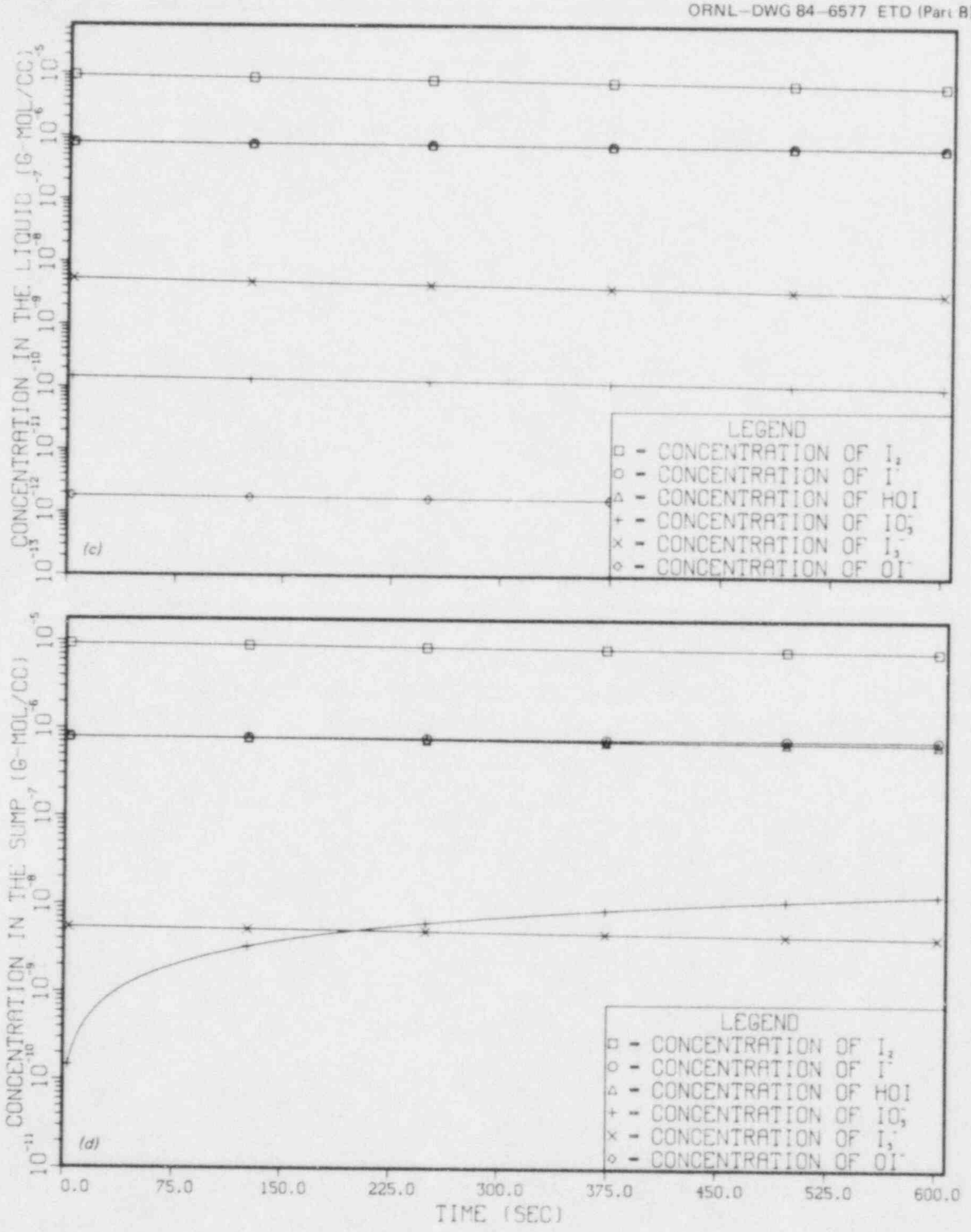


Fig. 62. (continued).

ORNL-DWG 84-6578 ETD (Part A)

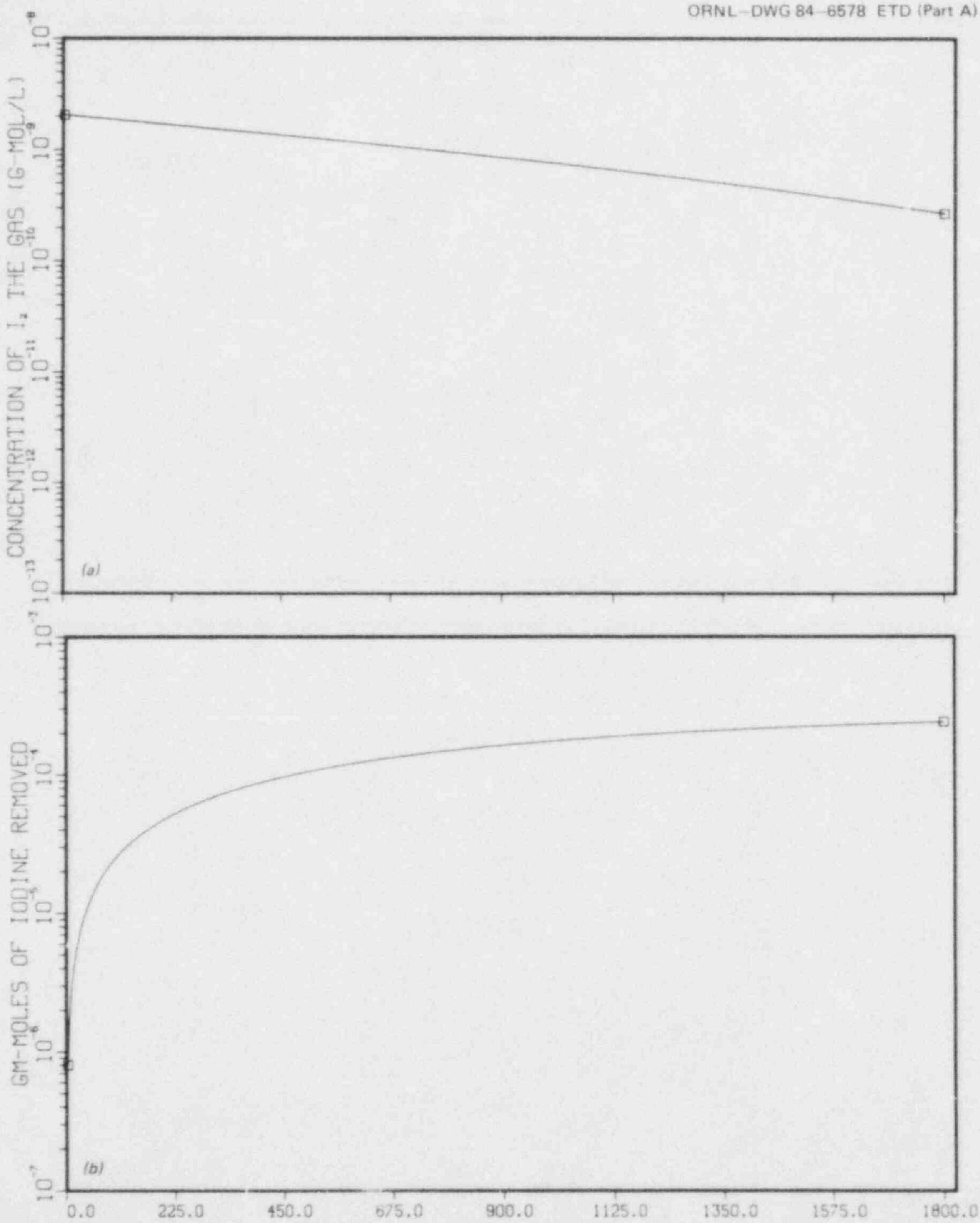


Fig. 63. Results of Spray Model for CSE run A-7 second spray period. Initial concentration of molecular iodine in the gas phase of 2.05×10^{-8} moles/liter and a buffered pH of 5.0 in the spray solution.

(a) Concentration of molecular iodine in the gas phase as a function of time.

(b) Number of moles of molecular iodine transferred as a function of time.

(c) Concentration of iodine species in the liquid drops as a function of time.

(d) Concentration of iodine species in the sump as a function of time.

ORNL–DWG 84–6578 ETD (Part B)

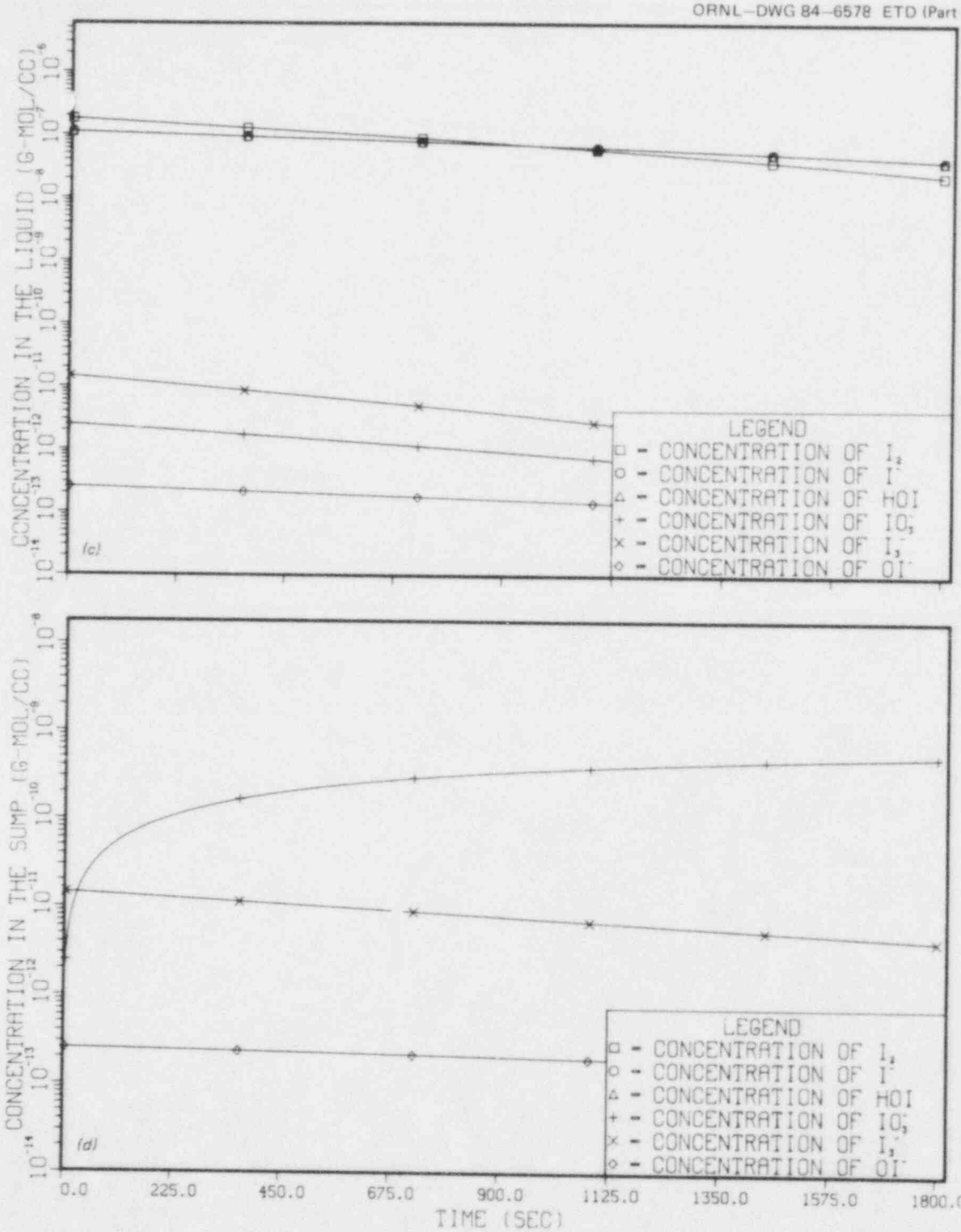


Fig. 63. (continued).

ORNL-DWG 84-6583 ETD (Part A)

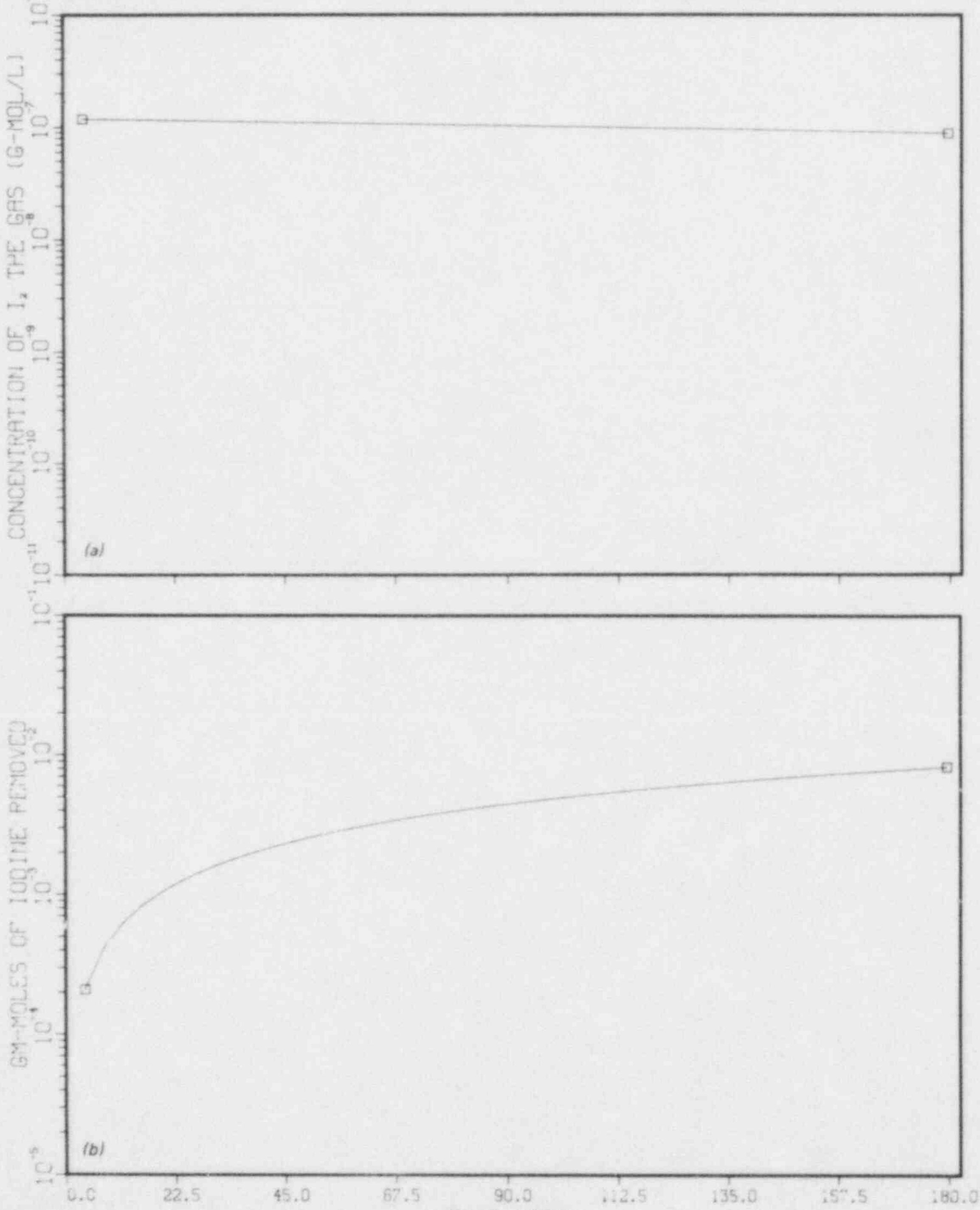


Fig. 64. Results of Spray Model for CSE run A-8 first spray period. Initial concentration of molecular iodine in the gas phase of 1.18×10^{-7} moles/liter and a buffered pH of 9.5 in the spray solution.

(a) Concentration of molecular iodine in the gas phase as a function of time.

(b) Number of moles of molecular iodine transferred as a function of time.

(c) Concentration of iodine species in the liquid drops as a function of time.

(d) Concentration of iodine species in the sump as a function of time.

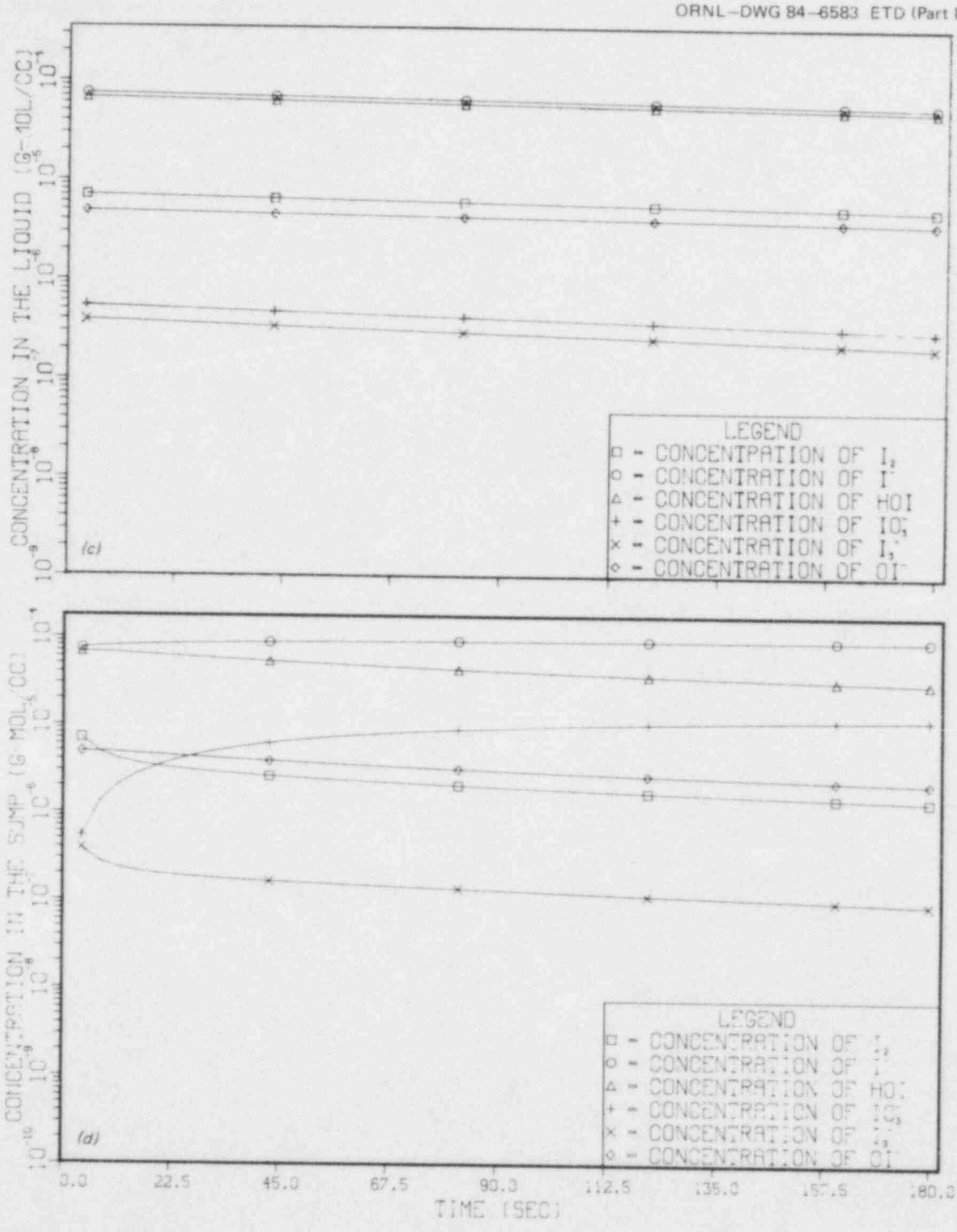


Fig. 64. (continued).

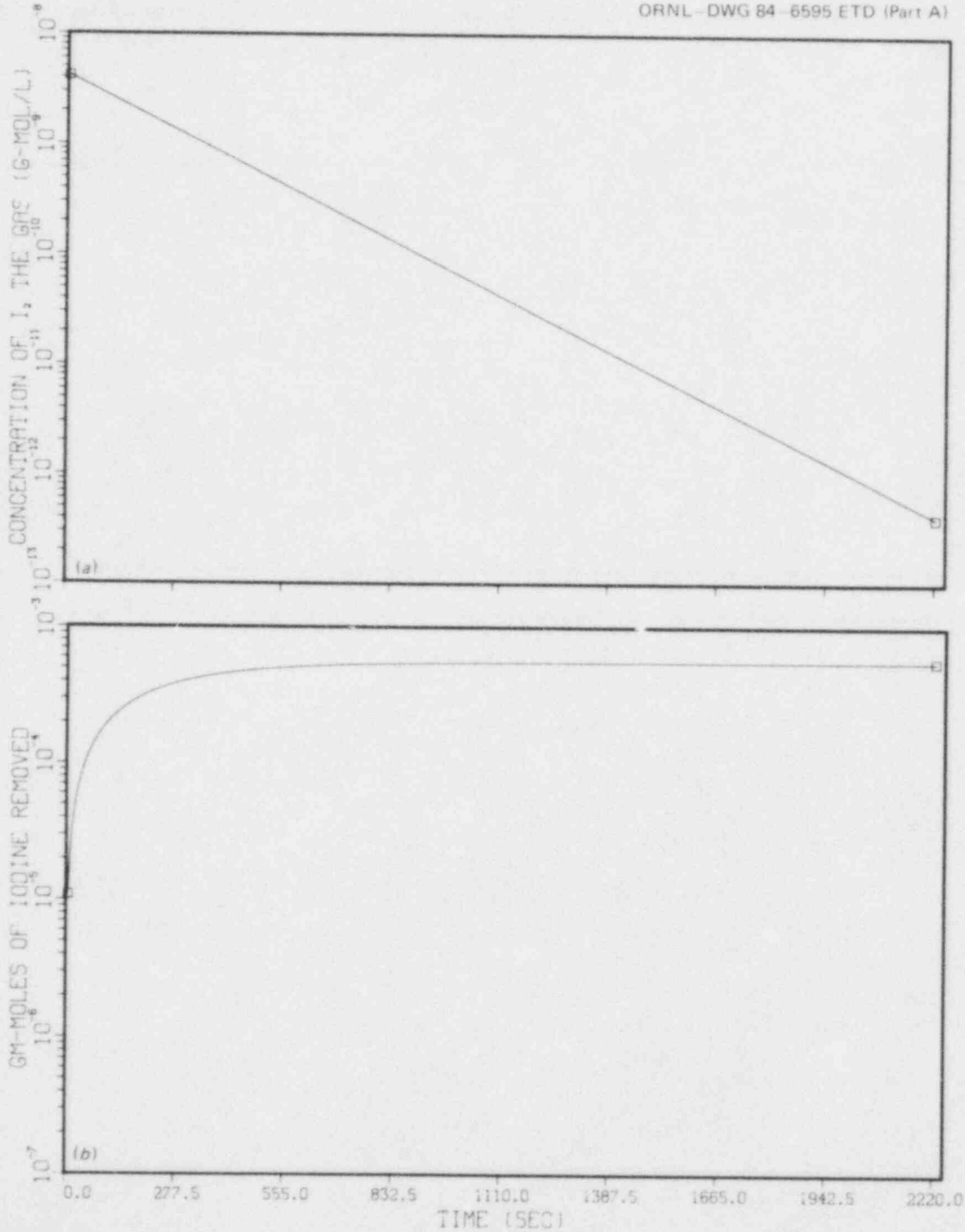


Fig. 65. Results of Spray Model for CSE run A-8 second spray period. Initial concentration of molecular iodine in the gas phase of 4.14×10^{-9} moles/liter and a buffered pH of 9.5 in the spray solution.

(a) Concentration of molecular iodine in the gas phase as a function of time.

(b) Number of moles of molecular iodine transferred as a function of time.

(c) Concentration of iodine species in the liquid drops as a function of time.

(d) Concentration of iodine species in the sump as a function of time.

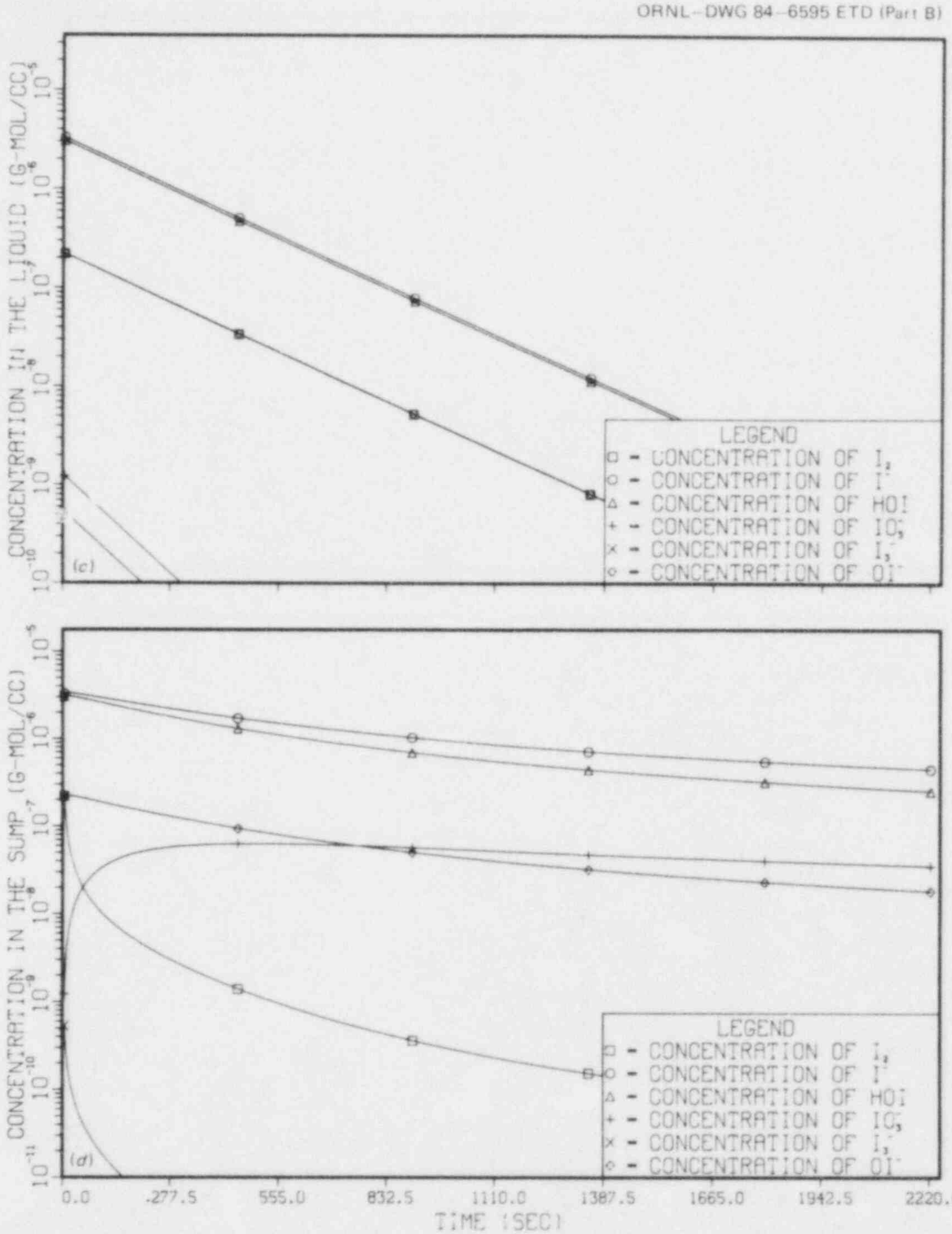


Fig. 65. (continued).

Spray flow rate = 12.8 gallons/minute = 48.5 liters/minute (full containment),
= 4.8 gallons/minute = 18.18 liters/minute (drywell area),
Spray time = 10 minutes,
Containment height = 15.4 meters,
Containment diameter = 3.35 meters.

For the First Spray:

Initial concentration of elemental iodine in the gas phase = 5×10^4 micrograms/cubic meter = 1.97×10^{-7} moles/liter,
Initial concentration of iodine in the drywell sump = 8.0×10^2 micrograms/cubic meter,
Initial volume of liquid in the drywell sump = 150 liters.

Results of the CSE tests are:

Final concentration of elemental iodine in the gas phase = 1.25×10^4 micrograms/cubic meter = 4.92×10^{-8} moles/liter,
Number of grams removed from the gas phase = 3.75×10^4 micrograms/liter * 15.4 meters * 8.8 square meters = 5.82×10^6 micrograms = 5.082 grams,
Final concentration in the drywell sump = 4×10^4 micrograms/liter,
Final volume in the sump = 331.8 liters,
Number of grams transferred to the liquid = (4×10^4 micrograms/liter * 331.8 liters) - (8×10^2 micrograms/liter * 150 liters) = 13.15×10^6 micrograms = 13.15 grams.

These calculations show the discrepancy between the number of grams of iodine removed from the gas phase, 5.082 grams, and the number grams of iodine transferred to the liquid, 13.15 grams. This discrepancy is discussed in Chapter 7.

Results of the Spray Model (for run A-3 first spray figure 56) is:

Final concentration of the gas phase = 2.4×10^4 micrograms/cubic meter = 9.45×10^{-8} moles/liter,
Number of grams of iodine removed from the gas and transferred to the liquid = 3.54 grams.

Relative Percent Difference is:

Gas phase,

$$\frac{(5.082 - 3.54)}{5.082} \times 100\% = 30.4\% ,$$

Liquid phase

$$\frac{(13.15 - 3.54)}{13.15} \times 100\% = 73.1\% .$$

Table 10 contains the results of the comparisons for all of the runs. The third or fourth spray periods are not included in the comparison because these periods are for a sodium thiosulfate spray solution or for recirculatory spray solutions. The sodium-thiosulfate changes the chemical kinetics and therefore, the model developed in this report should not be expected to be valid. However, recirculatory spray solutions can be used in the spray model if one knows the concentration of all of the species in the solution. The experimental data do not report the concentration of all of the species and since the liquid phase data are questionable (discussed in Chapter 7), and any results would be essentially meaningless. Therefore no further comparisons were attempted.

With a high initial concentration of molecular iodine in the gas, such as those seen during the first spray period, the spray model predicts the number of grams of iodine removed within a relative difference of between 13.8% and 68%. At low concentrations of molecular iodine in the gas, such as those seen during the second spray period, the spray model predicts the number of grams of iodine removed within a relative difference of -120.0% to 68.0% with the closest result having a difference of 7.7%. At high concentrations, the model always underpredicts the number of moles transferred as indicated by the experimental data. At low concentrations of molecular iodine in the gas, the model over-predicted the removal rate 4 out of 5 times when compared to the gas phase data. It should also be noted that the spray model never over-predicts the number of grams removed when compared to the experimental data for the liquid.

The only difference between the conditions of experimental runs A-3 and A-4 is the spray flow rate. The model responds quite adequately and, in fact, the difference in results decreases slightly. For experimental runs A-6, A-7, and A-8, the temperature and pressure of the gas are raised to approximately 397K and 3 atmospheres, respectively. The results of the spray model appear to have larger difference with the experimental data because the spray model does not contain calculations for heat transfer and the temperature of the drop always remain at its initial temperature of 298K. The properties of the liquid change with temperature and the kinetic rate constants will also change.

In run A-8, the drop size decreases to 770 microns. The model responds adequately and the error is most likely due to the higher temperature. It should be recalled that all of these results are produced with an input that assumes spherical drops. The drops are not spherical, but no information is available on the actual shape of the drops.

Comparing the new model to the previous models shows the new model has a better correlation with the experimental data than do the previous models. The data and the previous models are in terms of a removal rate constant and half lives of molecular iodine. The removal rate constant is expressed by Equation 2 of Chapter 1, Section 2, repeated here:

$$C = C_o \exp(-\lambda t) \qquad (2)$$

Table 10. Comparison of spray model to the CSE tests

CSE run	Spray period	Initial gas phase concentration (moles/liter)	CSE experimental results			Spray model's results		Relative percent difference between the gas phases
			Final gas phase concentration (moles/liter)	Grams removed from the gas phase	Grams transferred to the liquid phase	Final gas phase concentration (moles/liter)	Grams transferred from the gas to the liquid	
A-3	1st	1.97×10^{-7}	4.92×10^{-9}	5.082	13.15	9.50×10^{-8}	3.54	30.3
A-3	2nd	1.27×10^{-8}	2.89×10^{-10}	0.426	4.90	1.26×10^{-9}	0.393	7.7
A-4	1st	1.50×10^{-7}	1.97×10^{-9}	5.082	12.85	3.17×10^{-8}	4.07	19.9
A-4	2nd	7.88×10^{-10}	7.88 × 10-11	0.0244	1.124	6.61×10^{-12}	0.0269	-10.2
A-6	1st	8.67×10^{-9}	2.36×10^{-9}	2.900	11.10	1.40×10^{-8}	2.50	13.8
A-6	2nd	2.01×10^{-9}	1.10×10^{-9}	0.312	2.33	7.92×10^{-12}	0.0688	-120.5
A-7	1st	1.06×10^{-7}	3.27×10^{-9}	3.547	8.08	7.35×10^{-8}	1.14	68.0
A-7	2nd	2.05×10^{-9}	7.49×10^{-10}	0.0447	1.57	2.62×10^{-10}	0.0615	-37.6
A-8	1st	1.18×10^{-7}	5.12×10^{-9}	3.889	7.57	5.77×10^{-8}	2.12	45.5
A-8	2nd	4.14×10^{-9}	2.17×10^{-9}	0.0678	4.96	2.89×10^{-13}	0.143	-110.1

where

C_o = initial concentration of molecular iodine in the gas phase,
C = concentration of molecular iodine,
λ = removal rate constant, and
t = time.

Rearranging Equation 2 and solving for the removal rate constant:

$$\lambda = - \text{Ln } (C/C_o)/t \ . \tag{69}$$

The half life of molecular iodine is the period of time during which the concentration of molecular iodine in the gas phase decreases to one half of its initial concentration. The half life is determined by rearranging Equation 2 into:

$$t_{1/2} = - \text{Ln}(C/C_o)/\lambda = - \text{Ln}(1/2)/\lambda = 0.693/\lambda \tag{70}$$

Using these two equations, one can compare directly the experimental spray data and the results of the previous models in their existing form.

Note that the new spray model is not intended to determine a removal rate constant because removal rate constants tend to smooth out the data and can give false impressions since a logarithm is involved. The output of the new spray model is only put into this form to compare its results to the results of the existing models. The correct comparison would be to compare the number of moles removed or the resulting gas phase concentration.

Table 11 shows the comparison of the removal rate constant for the new model to that for the experimental data. As can be seen from Table 11, the new spray model always over-predicts the removal rate constant (under-predicts the removal rate) for the first spray period (high concentrations of molecular iodine). The absolute value difference for the new model is from 34.0% to 89.3% with an average difference of approximately 59.6%. One should notice that these differences do not have as wide a spread between the numbers as does the difference for the direct comparison of the number of grams of molecular iodine transferred to the liquid. This difference is due to the fact that the removal rate constant is calculated from a logarithm which smooths out the error. It is far more realistic to use the number of grams of molecular iodine removed for comparison.

A comparison of the results of the previous spray models is shown is Table 12. Note that the "realistic model" is the name given to this model when it was first developed for inclusion in WASH-1329[2] and does not imply that it is the best model.

It is quite obvious that from Table 12 that for the first spray period of runs A-3, A-4, A-6, and A-8, the new spray model is not as accurate as some of the older models. Since the old models are not a function of the gas phase concentration of iodine and the parameters used in the old model for the first spray period and the second spray

Table 11. Comparison of removal rate constant for spray model against CSE tests

CSE run	Spray period	Initial gas phase concentration (moles/liter)	CSE tests results			Spray model's results			Relative percent difference[a] between removal rate constants
			Final gas phase concentration (moles/liter)	Removal rate constant, λ (min^{-1})	Half life t1/2 (min)	Final gas phase concentration (moles/liter)	Removal rate constant, λ (min^{-1})	Half life t1/2 (min)	
A-3	1st	1.97×10^{-7}	4.92×10^{-8}	0.139	5.0	9.50×10^{-8}	0.074	9.5	47.1
A-3	2nd	1.29×10^{-8}	2.89×10^{-10}	0.126	5.5	1.26×10^{-9}	0.077	9.0	38.9
A-4	1st	1.50×10^{-7}	1.97×10^{-9}	0.495	1.4	3.17×10^{-8}	0.155	4.47	34.0
A-4	2nd	7.88×10^{-10}	7.88×10^{-11}	0.077	9.0	6.61×10^{-12}	0.159	4.35	107.0
A-6	1st	8.67×10^{-8}	2.36×10^{-9}	0.365	1.9	1.40×10^{-8}	0.182	3.8	50.1
A-6	2nd	2.01×10^{-9}	1.10×10^{-9}	0.022	32.0	7.92×10^{-12}	0.184	3.75	739.0
A-7	1st	1.06×10^{-7}	3.27×10^{-9}	0.347	2.0	7.35×10^{-8}	0.037	18.7	89.3
A-7	2nd	2.05×10^{-9}	7.49×10^{-10}	0.033	21.0	2.62×10^{-10}	0.068	9.33	107.0
A-8	1st	1.18×10^{-7}	5.12×10^{-9}	1.08	0.64	5.77×10^{-8}	0.239	2.67	77.4
A-8	2nd	4.14×10^{-9}	2.17×10^{-9}	0.017	40.0	2.89×10^{-13}	0.257	2.89	1307.0

[a]Difference = $\frac{|(\lambda_{CSE} - \lambda_{SPRAY})|}{\lambda_{CSE}} \times 100\%$.

Table 12. Comparison of removal rate constant for spray model against previous models

CSE run number	Spray period	Experimental λ, min^{-1}	"Realistic"[a] model λ, min^{-1}	Stagnant[b] film model λ, min^{-1}	Stagnant[c] drop model λ, min^{-1}	CSE model[d] λ, min^{-1}	New model λ, min^{-1}
A-3	1st	0.139	0.102	0.027	0.053	0.109	0.074
	2nd	0.126	0.102	0.027	0.053	0.109	0.077
A-4	1st	0.495	0.39	0.093	0.195	0.408	0.155
	2nd	0.077	0.39	0.093	0.195	0.408	0.159
A-6	1st	0.365	0.34	0.202	0.235	0.365	0.182
	2nd	0.022	0.34	0.202	0.235	0.365	0.184
A-7	1st	0.347	*e*	*e*	*e*	*e*	0.037
	2nd	0.033	*e*	*e*	*e*	*e*	0.068
A-8	1st	1.08	1.02	0.483	0.527	0.978	0.239
	2nd	0.017	1.02	0.483	0.527	0.978	0.257

[a] Equation 6 with PC = 10^5.

[b] Equation 5 with PC = 5000.

[c] Equation 4 with PC = 5000.

[d] Equation 7.

[e] Published results not found.

period are the same. The removal rate constant predicted by the old models would be the same for the first and second spray periods. The new model would predict results closer to the spray tests than would the "realistic" model for the second spray period. Although the "realistic" model does predict close results for the first spray period, it uses an effective partition coefficient of 100,000. For a drop fall height of 15.4 meters, the contact time of the drop with the gas phase is only 3.9 seconds and the effective partition coefficient at the conditions would only be approximately 2200. An effective partition coefficient of 100,000 would not be reached until approximately 10 days at a pH of 9.5. So this effective partition coefficient of 100,000 would not be reached until approximately 10 days at a pH of 9.5, a temperature of 298 K, and an initial concentration of 10^{-7} g-atoms/L or approximately 15 min at 373 K and 10^{-7} g-atoms/L. So this effective partition coefficient consists of a true effective partition coefficient times an empirical factor. It is believed that this effective partition coefficient was picked so as to best describe the results for the first spray period. If a situation would arise for the need of the "realistic" spray model and it did not occur in this same vessel used in the CSE tests and under exactly the same conditions, the correction factor may be wrong.

The CSE model is a gas-film controlled model and is compared to tests maybe with a buffered high pH. The controlling resistance to mass transfer for iodine would be gas-film controlled under these conditions because the reactions quickly remove the molecular iodine in the liquid. However, when the pH is buffered at a low pH or when the pH is unbuffered, there will be significant resistance to mass transfer in both phases. BWRs use ordinary water for their sprays, so there will be significant resistance to mass transfer is both phases. Therefore, the CSE model would give incorrect results for BWRs and any other system not buffered at a high pH.

Since the iodine hydrolysis reactions are included in the new spray model, they can determine internally when the reactions play an important role in the mass transfer, and the new spray model should be valid for any conditions. The new spray model appears to give better results at low concentrations than for high concentrations of iodine in the gas phase. The difference between the experimental data and the new spray model can be caused by incorrect correlations for the mass transfer coefficients, incorrect data for the molecular iodine partition coefficient, incorrect expressions for the iodine hydrolysis reactions, or from incorrect reaction rate constants. But much of the difference is believed to be in the experimental spray data.

9. SUMMARY, CONCLUSIONS, AND RECOMMENDATIONS

9.1 Summary

A new model has been developed for predicting the rate at which gaseous molecular iodine is absorbed by water sprays. The model is a quasi-steady state mass transfer model that includes the iodine hydrolysis reactions. The spray model was developed to determine numerically the influence of the iodine hydrolysis reaction on the mass transfer rates. The spray model is used to determine if inclusion of a representation of the iodine hydrolysis reactions increases the understanding of what is occurring and increases the realism of the actual process. The spray model is also used to see if the new models provide an increase in accuracy for the removal of gaseous iodine. The parameters of the spray model are the spray drop size, initial concentration of molecular iodine in the gas phase, the initial concentration of all of the iodine hydrolysis species (including pH), the temperature of the gas, the temperature of the liquid, the pressure, whether the spray solution is buffered or unbuffered, the spray flow rate, containment diameter, and containment height (drop fall height).

Three other models have also been developed; these are kinetic, drop, and wall spray models. The kinetic model simulates the solution to the equations to the iodine hydrolysis reactions as a function of time. The drop model simulates the absorption of gaseous iodine by a single water droplet. The drop model has a mass transfer with reaction algorithm and is the base model for the spray model. The wall-spray model contains the spray model algorithm plus a falling-liquid film algorithm to simulate the removal of gaseous iodine by the water on the walls. The results of the wall-spray model are not significantly different from the results of the spray model and therefore the significantly longer computational time necessary to use the wall-spray model is not warranted.

The spray model shows a difference of -120.5% to 68.0% compared to the measured data of the Containment Systems Experiments with the closest result being within 7.7% of the experimental data. Some of the difference is believed to be due to error in the measured data from the experiment caused by the sampling techniques used and the fact that these tests are large scale with many removal processes occurring simultaneously. Molecular iodine is absorbed on paint, piping, insulation and particulates as well as on the spray drops. With all of these processes occurring simultaneously, it is extremely difficult to separate the contribution of the drops to iodine removal from the overall removed. Since litteral interpretation of the experimental data show that twice as much iodine is transferred to the liquid phase as is removed from the gas phase, it is obvious that there are significant experimental errors present.

Other sources for the difference between the calculated results and the experimental data of error undoubtedly result from limitations in the spray model itself. The spray model does not include any representation of enhanced mass transfer during drop formation, and it has

been shown by Simpson[19] that significantly higher mass transfer rates do occur during drop formation. Another source of difficulty is the unknown sphericity of the drops of the experiment. The new spray model has the ability to handle non-spherical drops, but there is no information on the sphericity for the spray drops and Clift[12] indicates that drops of the size used in these tests are significantly non-spherical. Using non-spherical drops would increase the rate of mass transfer by increasing the surface area of the drops.

The spray model also does not consider heat transfer. Temperature changes in both the gas and liquid phases can alter the rate of mass transfer. The difference in results between the spray model and the experimental data increases when the initial temperature of the gas is not the same as the temperature of the liquid. Since there are no heat transfer calculations in the model, the gas and liquid phases are assumed to remain at the same temperature throughout the simulation.

9.2 Conclusions

The following conclusions can be made about this work:

1. The iodine hydrolysis reactions in some cases have a major influence on the removal of gaseous molecular iodine by water droplets and thus should be included in a model. The iodine hydrolysis reactions have their largest effect on the rate of removal of molecular iodine when the spray solution is buffered at a high pH. The iodine hydrolysis reactions have a small effect on the rate of removal of molecular iodine when the spray solution is unbuffered at any pH or when the spray solution is buffered at a low pH. It is also essential to account for the iodine hydrolysis reactions whenever the spray solution is to be recirculated because one must know the concentration of all of the iodine hydrolysis reaction species in order to determine when molecular iodine is stripped form the spray solution back into the gas phase.

2. The new spray model is based upon theory, acceptable correlations and experimental data (used only for the physical data of the species involved). There is no unknown variables that must be known to "fit" the data. Whereas the effective partition coefficient in the "realistic" model (Eq. 7 with an effective partition coefficient of 100,000) appears to have been empirically "fitted" to the Containment Systems Experiments.[3] Therefore, it would be unwise to extrapolate the results of the "realistic" model to other conditions or situations. This is proven if one compares the results of the "realistic" model to the experimental data for the second spray periods. The new spray model also provides the essential information about the liquid phase so that it can be used for recirculatory sprays. No other spray model provides this information nor could these old models be used with any confidence for recirculatory sprays.

3. The new spray model's results compare better to the CSE results for low concentrations of molecular iodine in the gas phase, the second spray periods, than does the "realistic model but gives worse results at high concentrations of molecular iodine in the gas phase. The reason

for the "realistic" model's results are closer to the tests at high concentrations of molecular iodine in the gas phase, the first spray periods, is because the effective partition coefficient appears to have been empirically "fit" to the first spray period. Therefore, the "realistic" model should give closer results for the first spray period, but it also gives extremely inaccurate result for the second spray periods. It should also be pointed out that in any conceivable accident, radiation would be present and could alter results based on hydrolysis alone by generating molecular iodine within the drops and by changing the pH in unbuffered sprays due to the formation of nitric acid.

9.3 Recommendations

It is recommended that all of the models: kinetic, drop, spray, and wall-spray models, be tested more extensively. It is recommended that both heat transfer and mass transfer during drop formation be incorporated into the spray model.[19] Adding a representation of heat transfer would probably make the most significant improvement to the models and allow better comparison to experimental data taken from tests in which a temperature difference exists between the gas and liquid phases. The most important recommendation is that new smaller scale tests, which are more highly controlled, should be conducted. Presently there is a greater need for new data to which the results of these new models could be compared than there is a need for a more sophisticated model. Smaller scale experimental tests under better controlled conditions are suggested in which the only process for the removal of gaseous iodine would be by water drops or sprays. A small scale drop test could also be useful. Since the spray model is based upon the drop model, the drop model should be tested to see if it is correct. The drop model must simulate a drop falling through gaseous iodine correctly; if not, then both the spray model and the wall-spray model would be incorrect.

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Appendix A

NUMERICAL TECHNIQUE

All of the models involve the iodine hydrolysis reactions and an efficient numerical integration technique must be used. The kinetic model numerically integrates the iodine hydrolysis reactions with respect to time. The drop, spray and wall-spray models all contain mass transfer of molecular iodine to the liquid and the iodine hydrolysis reactions occurring in the liquid drop. Therefore, in all of the models the iodine hydrolysis reactions must be integrated.

The iodine hydrolysis reactions are integrated by a Runge-Kutta-Felhburg, RKF, 5(4) order numerical integration routine.[11] RKF 5(4) has is a fifth order Runge-Kutta routine with a fourth order routine imbedded in it. The RKF routine is a single step method with error control. To save computer calculation time the routine in the model only contains the parts of the RKF routine which are necessary to integrate these equations and the absolute error control has been replaced by a relative error control to improve accuracy and computer time. The error control is possible by comparing the difference between the two orders. The model requires as input the number of equations to integrate. For a buffered solution, there are four equations to numerically integrate. Equations 23, 24, and 25 are assumed to come to equilibrium instantaneously and since the hydrogen ion concentrations will not change, one would have to integrate Equations 26 through 29. For unbuffered solutions the pH would change, so Equation 31 would have to be integrated, so five equations would have to be integrated. Therefore, for a buffered solution the input parameter IN would be four and for an unbuffered solution IN would be equal to five.

Other numerical integration routines have been tried such as DGEAR and DVERK from the International Mathematics and Statistics Library, IMSL, and LSODE from Corlib. Neither of the IMSL routines would get started because the step size would drop below the accuracy of the machine. This is most likely due to the complexity of the differential equations. LSODE is a Gear's multistep integration routine. Gear's method works extremely well for the kinetic model. In fact LSODE works better in the kinetic model for longer periods of time. This is the routine that Bell[7] used. When mass transfer is included this routine becomes extremely slow, taking almost 10 times more computer time than does the RKF routine. This is because LSODE is a multistep method and each time mass transfer occurs a new concentration of molecular iodine is determined and the system must start over. So the RKF method was chosen because error can be minimized and efficiency can be achieved.

Appendix B

KINETIC MODEL, SAMPLE INPUT AND OUTPUT

```
C*****************************************************************************
C
C     KINETIC MODEL
C
C     M. F. ALBERT
C
C     THE KINETIC SIMULATES THE AQUEOUS IODINE HYDROLYSIS REACTIONS.
C     REACTIONS 4, 5 AND 6 (EQUATIONS 23, 24, AND 25) ARE ASSUMED TO
C     COME  TO EQUILIBRIUM .  THE KINETIC MODEL NUMERICALLY INTEGRATES
C     EQUATIONS 25 THROUGH 31 WITH A RUNGE-KUTTA-FELHBURG 5(4) ROUTINE.
C     SUBROUTINE FUNCTN AND ITTER ARE CALLED FROM THIS MAIN PROGRAM.
C     SUBROUTINE FUNCTN CONTAINS THE EQUATIONS TO BE INTEGRATED.
C     SUBROUTINE ITTER FINDS THE ROOT TO THE EQUILIBRIUM EQUATION OF
C     EQUATION 23 BY A SECANT METHOD.  THIS PROGRAM IS DESIGNED TO RUN
C     ON A PDP-10 COMPUTER BUT SHOULD BE EASILY CONVERTED TO RUN ON ANY
C     FORTRAN COMPUTER.
C
C******************************************************************************
C
C
      IMPLICIT DOUBLE PRECISION (A-H,K-Z)
      IMPLICIT INTEGER (I-J)
C
C
      DIMENSION W(8),WOLD(8),K1(7),K2(7),K3(7),R(7),WB(7),
     1     DELTA(7),WES(7),F(7),K4(7),K5(7),K6(7),TOL(7)
C
C
      READ(58,*)A,B,HMIN,HMAX,IN
      READ(49,*)TOLER,TEMPL
C
C
11    FORMAT('    N       TIME            I2             I-                HOI
     1    IO3-            H+             IO-            I3-       STEP SIZE'
     2,/)
21    FORMAT('STEP SIZE BELOW STEP MIN',D15.7)
22    FORMAT(I5,9D13.7)
25    FORMAT(I6)
C
      WRITE(50,11)
C
C
C     READ IN INITIAL CONDITIONS
C
      DO 20 J=1,7
      READ(58,*)WOLD(J)
20    CONTINUE
C
      TOLD=A
      Q=1.0D-1
      H=1.0D-2
C
      WRITE(50,22)I,TOLD,WOLD(1),WOLD(2),WOLD(3),WOLD(4),WOLD(5),WOLD(6)
     1              ,WOLD(7),H
C
C     CALCULATE THE EQUILIBRIUM CONSTANST K4,K5,K6
C
      DENLIQ=6.0252247D-9*TEMPL**3-9.1329604D-6*TEMPL**2+3.573572D-3*TEM
     1PL+5.8358882D-1
      RK6=-4.098D00-3245.2D00/TEMPL+2.2363D5/(TEMPL**2)-3.984D7/(TEMPL**
     13)+(13.957D00-1262.3D00/TEMPL+8.5641D5/(TEMPL**2))*DLOG(DENLIQ)
      RK6=10**(RK6)
C
```

```
      RK5=10**(2800.48D00+0.7335D00*TEMPL-80670.0D00/TEMPL
     1-1115.1D00*DLOG10(TEMPL))
C
      RK4=DEXP(3727.86D00/TEMPL-11.6326D00+0.0192212D00*TEMPL)
C
      WOLD(8)=RK6/WOLD(5)
C
C     BEGIN THE RUNGE-KUTTA-FEHLBERG ROUTINE
C
C
C     CALCULATE K'S
C
1     DO 30 J=1,IN
       W(J)=WOLD(J)
30    CONTINUE
C
      CALL FUNCTN(W,WOLD,F,IN)
C
      DO 40 J=1,IN
       K1(J)=H*F(J)
40    CONTINUE
C
      DO 50 J=1,IN
       W(J)=WOLD(J)+K1(J)/4.0D00
50    CONTINUE
C
      CALL FUNCTN(W,WOLD,F,IN)
C
      DO 60 J=1,IN
       K2(J)=H*F(J)
60    CONTINUE
C
      DO 80 J=1,IN
       W(J)=WOLD(J)+3.0D00*K1(J)/3.2D1+9.0D00*K2(J)/3.2D1
80    CONTINUE
C
      CALL FUNCTN(W,WOLD,F,IN)
C
      DO 90 J=1,IN
       K3(J)=H*F(J)
90    CONTINUE
C
      DO 110 J=1,IN
       W(J)=WOLD(J)+1.932D3*K1(J)/2.197D3-7.2D3*K2(J)/2.197D3
     1       +7.296D3*K3(J)/2.197D3
110   CONTINUE
C
      CALL FUNCTN(W,WOLD,F,IN)
C
      DO 120 J=1,IN
       K4(J)=H*F(J)
120   CONTINUE
C
      DO 130 J=1,IN
       W(J)=WOLD(J)+4.39D2*K1(J)/2.16D2-8.0D00*K2(J)+3.68D3*K3(J)/5.13D2
     1       -8.45D2*K4(J)/4.104D3
130   CONTINUE
C
      CALL FUNCTN(W,WOLD,F,IN)
C
      DO 140 J=1,IN
       K5(J)=H*F(J)
140   CONTINUE
C
      DO 150 J=1,IN
       W(J)=WOLD(J)-8.D00*K1(J)/2.7D1+2.D00*K2(J)-3.544D3*K3(J)/2.565D3
```

```
     1      +1.859D3*K4(J)/4.104D3-1.1D1*K5(J)/4.0D1
150   CONTINUE
C
      CALL FUNCTN(W,WOLD,F,IN)
C
      DO 160 J=1,IN
       K6(J)=H*F(J)
160   CONTINUE
C
C      DETERMINE THE NEW CONCENTRATION OF ALL OF THE IODINE HYDROLYSIS
C      SPECIES AND CHECK THE ERROR
C
      DO 100 J=1,IN
       WB(J)=WOLD(J)+1.6D1*K1(J)/1.35D2+6.656D3*K3(J)/1.2825D4+
     1       2.8561D4*K4(J)/5.643D4-9.0D00*K5(J)/5.0D1+2.0D00*K6(J)/5.5D1
       R(J)=ABS(K1(J)/3.6D2-1.28D2*K3(J)/4.275D3-2.197D3*K4(J)/7.524D4
     1          +K5(J)/5.0D1+2.0D00*K6(J)/5.5D1)/H
       TOL(J)=ABS(WB(J)*TOLER)
       DELTA(J)=0.84*(TOL(J)/R(J))**0.25
100   CONTINUE
C
      DO 500 J=1,IN
       IF(R(J) .GT. TOL(J))GOTO 900
500   CONTINUE
C
      DO 510 J=1,IN
       WOLD(J)=WB(J)
510   CONTINUE
C
C     DETERMINE THE EQUILIBRIUM CONCENTRATIONS FOR EQUATIONS 23, 24 AND
C     25
C
      BB=-1.0D00-(WOLD(2)+WOLD(1))*RK4
      C=WOLD(2)*WOLD(1)*RK4-WOLD(7)
      D=-BB/(2.0D00*RK4)
      E=((BB**2.0D00-4.0D00*RK4*C)**0.5D00)/(2.0D00*RK4)
      V=D-E
C
      IF(V .LT. 1.0D-18)CALL ITTER(WOLD,RK4,C,V)
C
      WOLD(7)=WOLD(7)+V
      WOLD(1)=WOLD(1)-V
      WOLD(2)=WOLD(2)-V
C
      IF(IN .EQ. 4)GOTO 600
      RR=WOLD(6)+WOLD(5)+RK5
      S=-RK5*WOLD(3)+WOLD(6)*WOLD(5)
      M=(-RR+(RR*RR-4.0D00*S)**0.5)/2.0D00
      WOLD(5)=WOLD(5)+M
      GOTO 605
C
600   M=(RK5*WOLD(3)-WOLD(6)*WOLD(5))/(WOLD(5)+RK5)
C
605   WOLD(6)=WOLD(6)+M
      WOLD(3)=WOLD(3)-M
C
      IF(IN .EQ. 4)GOTO 615
C
      U=WOLD(8)*WOLD(5)-RK6
      VV=WOLD(8)+WOLD(5)
      X=(-VV+(VV*VV-4.0D00*U)**0.5)/2.0D00
      WOLD(5)=WOLD(5)+X
      WOLD(8)=WOLD(8)+X
C
615   I=I+1
      TOLD=TOLD+H
```

```
C
      WRITE(50,22)I,TOLD,WOLD(1),WOLD(2),WOLD(3),WOLD(4),WOLD(5),
     1            WOLD(6),WOLD(7),H
C
      DEL=DELTA(1)
C
      IF(IN .EQ. 1)GOTO 905
C
      DO 520 J=2,IN
       IF(DEL .LT. DELTA(J))GOTO 520
       DEL=DELTA(J)
520   CONTINUE
C
      GOTO 905
C
C     DETERMINE NEW STEP SIZE
C
900   DEL=DELTA(J)
C
905   IF(DEL .GT. Q)GOTO 910
      HNEW=Q*H
      GOTO 1000
C
910   IF(DEL .LT. 4.0)GOTO 920
      HNEW=4.0D00*H
      GOTO 1000
C
920   HNEW=DEL*H
C
C     CHECK NEW STEP SIZE WITH MAX AND MIN STEP SIZE
C
1000  IF (HNEW .LT. HMAX)GOTO 930
      HNEW=HMAX
C
930   IF (HNEW .LT. HMIN)GOTO 1111
      LEFT=B-TOLD-HNEW
C
      IF(LEFT .GT. 0.0)GOTO 5000
      HNEW=B-TOLD
C
5000  H=HNEW
      IF(TOLD .GE. B)GOTO 999
      GOTO 1
C
C
1111  WRITE(40,21)HNEW
999   WRITE(23,25)I,IN
      STOP
      END
```

```
C***********************************************************************
C
C      SUBROUTINE FUNCTN
C
C      THIS SUBROUTINE CONTAINS THE DIFFERENTIAL EQUATIONS (KINETIC RATE
C      EQUATIONS) TO BE INTEGRATED.  THIS SUBROUTINE IS CALLED FROM THE
C      RUNGE-KUTTA-FELHBURG INTEGRATION ROUTINE IN THE KINETIC, DROP,
C      SPRAY AND WALL-SPRAY MODELS.
C
C***********************************************************************
C
      SUBROUTINE FUNCTN (W,WOLD,F,IN)
C
      IMPLICIT DOUBLE PRECISION(A-H,K-Z)
      IMPLICIT INTEGER(I-J)
C
      DIMENSION W(8),WOLD(8),F(7)
C
      IF(IN .EQ. 5)GOTO 5
C
      W(5)=WOLD(5)
5     W(6)=WOLD(6)
C
      RK1=3.0D00
      RKR1=4.4D12
      RK20=2.5D02
      RK21=1.2D02
      RKR2=3.0D08
      RKP3=9.35D-8
C
      R1=RK1*W(1)
      RR1=RKR1*W(2)*W(3)*W(5)
      R20=RK20*W(3)**2.0D00
      R21=RK21*W(3)*W(6)
      RR2=RKR2*W(4)*W(2)**2.0D00*W(5)**2.0D00
      RP3=RKP3*W(5)*W(2)
C
      F(1)=-R1+RR1+5.0D-1*RP3
      F(2)=R1-RR1+2.0D00*(R20+R21)/3.0D00-2.0D00*RR2-RP3
      F(3)=R1-RR1-R20-R21+3.0D00*RR2
      F(4)=(R20+R21)/3.0D00-RR2
C
      IF (IN .EQ. 5)GOTO 10
C
      F(5)=0.0D00
      GOTO 11
C
10    F(5)=R1-RR1+R20+R21-3.0D00*RR2-4.0D00*RP3
C
11    F(6)=0.0D00
      F(7)=0.0D00
C
      RETURN
C
      END
```

```
C*********************************************************************
C
C     SUBROUTINE ITTER
C
C     THIS SUBROUTINE FINDS THE ROOT TO THE QUADRATIC EQUILIBRIUM
C     EQUATION FOR THE FORMATION REACTION OF TRI-IODIDE, I3- (EQUATION
C     23).  A SECANT METHOD IS THE ROUTINE USED TO FIND THE ROOT.  THIS
C     METHOD IS CALLED WHENEVER THE QUADRATIC FORMULA RESULTS IN LESS
C     THAN APPROXIMATELY THREE SIGNIFICANT FIGURES.  THIS SUBROUTINE
C     IS CALLED BY THE PROGRAMS KINETIC, DROP, SPRAY AND WALL-SPRAY.
C
C*********************************************************************
C
      SUBROUTINE ITTER(WOLD,RK4,C,V)
C
      IMPLICIT DOUBLE PRECISION (A-H,L-Z)
      IMPLICIT INTEGER (I-K)
C
      DIMENSION WOLD(7),W(7)
C
      P0=1.0D-16
      P1=1.0D-18
C
      Q0=C-RK4*P0*P0-P0*RK4*(WOLD(1)+WOLD(2))-P0
5     Q1=C-RK4*P1*P1-P1*RK4*(WOLD(1)+WOLD(2))-P1
C
      NEW=P1-Q1*(P1-P0)/(Q1-Q0)
C
      CHECK=ABS(NEW-P1)/P1
C
11    IF (CHECK .LT. 1.0D-4) GOTO 10
C
      P0=P1
      Q0=Q1
      P1=NEW
      GOTO 5
C
10    V=NEW
C
      RETURN
C
      END
```

Kinetic Model sample input:

A = 0.0	WOLD(1) = 1.0×10^{-3}
B = 15.0	WOLD(2) = 0.0
HMIN = 1.0×10^{-10}	WOLD(3) = 0.0
HMAX = 1.0×10^{2}	WOLD(4) = 0.0
IN = 4	WOLD(5) = 1.0×10^{-9}
TOLER = 1.0×10^{-4}	WOLD(6) = 0.0
TEMPL = 298 K	WOLD(7) = 0.0

N	TIME	I2	I-	UOI	IC3-	H+	IO-	I3-	STEP SIZE
0	.00000000D+00	.10000000D-02	.10000000D+00	.00000000D+00	.00000000D+00	.10000000D-08	.00000000D+00	.00000000D+00	.10000000D-01
1	.15072940D-02	.99350270D-03	.26059550D-05	.44101910D-05	.85320550D-12	.10000000D-08	.10143440D-06	.19056750D-05	.15072540D-02
2	.28597530D-02	.98608250D-03	.48553050D-05	.81576510D-05	.53974050D-11	.10000000D-08	.18854600D-06	.35309190D-05	.13024690D-02
3	.48671490D-02	.97547520D-03	.84056670D-05	.14139900D-04	.27761500D-10	.10000000D-08	.32521780D-06	.60595530D-05	.20573660D-02
4	.79551540D-02	.96673910D-03	.13727010D-04	.22565260D-04	.11587450D-09	.10000000D-08	.52820090D-06	.97670450D-05	.30880050D-02
5	.12383560D-01	.94695720D-03	.21335070D-04	.35424430D-04	.44558320D-09	.10000000D-08	.81476160D-06	.14902330D-04	.44284050D-02
6	.18486190D-01	.92499460D-03	.31783930D-04	.52212970D-04	.14532370D-08	.10000000D-08	.12008980D-05	.21637200D-04	.61026300D-02
7	.26602690D-01	.89442650D-03	.45576120D-04	.73859260D-04	.42189440D-08	.10000000D-08	.16587630D-05	.30002800D-04	.81165650D-02
8	.37056050D-01	.85722130D-03	.62135070D-04	.10059900D-03	.11023580D-07	.10000000D-08	.23137780D-05	.39832850D-04	.10453350D-01
9	.50129570D-01	.81287780D-03	.84700680D-04	.13226470D-03	.26157720D-07	.10000000D-08	.30420880D-05	.50736500D-04	.13073530D-01
10	.66048830D-01	.76561760D-03	.11025170D-03	.16822420D-03	.56792650D-07	.10000000D-08	.38691570D-05	.62125660D-04	.15919260D-01
11	.84973960D-01	.71419390D-03	.13944050D-03	.20739960D-03	.11362140D-06	.10000000D-08	.47701680D-05	.73296430D-04	.18925030D-01
12	.10700610D+00	.66172620D-03	.17157300D-03	.24836730D-03	.21090440D-06	.10000000D-08	.57124490D-05	.83561290D-04	.22032280D-01
13	.13221130D+00	.61032400D-03	.20565110D-03	.28958100D-03	.36576610D-06	.10000000D-08	.66594440D-05	.92378180D-04	.25205150D-01
14	.16065460D+00	.56183730D-03	.24047650D-03	.32935080D-03	.59689040D-06	.10000000D-08	.75752070D-05	.99439980D-04	.28443300D-01
15	.19244330D+00	.51766080D-03	.27475360D-03	.36644570D-03	.92309540D-06	.10000000D-08	.84282520D-05	.10469590D-03	.31788380D-01
16	.22776700D+00	.47867030D-03	.30743510D-03	.39973950D-03	.13622750D-05	.10000000D-08	.91940080D-05	.10830970D-03	.35324020D-01
17	.26693950D+00	.44525850D-03	.33743500D-03	.42851050D-03	.19305570D-05	.10000000D-08	.98557420D-05	.11058220D-03	.39172470D-01
18	.31043270D+00	.41783140D-03	.36412080D-03	.45236140D-03	.26447500D-05	.10000000D-08	.10404310D-04	.11186870D-03	.43493180D-01
19	.35891990D+00	.39490990D-03	.38710240D-03	.47118360D-03	.35168710D-05	.10000000D-08	.10837220D-04	.11251270D-03	.48487240D-01
20	.41333130D+00	.37722280D-03	.40630650D-03	.48510460D-03	.45699550D-05	.10000000D-08	.11157410D-04	.11280530D-03	.54411270D-01
21	.47493640D+00	.36377700D-03	.42152600D-03	.49443110D-03	.58178720D-05	.10000000D-08	.11371920D-04	.11296640D-03	.61605100D-01
22	.54095180D+00	.35440940D-03	.43371360D-03	.49939170D-03	.71935920D-05	.10000000D-08	.11486010D-04	.11313210D-03	.66022450D-01
23	.61301970D+00	.34789950D-03	.44278860D-03	.50106660D-03	.87144450D-05	.10000000D-08	.11524530D-04	.11337490D-03	.72060510D-01
24	.69282940D+00	.34336140D-03	.44955840D-03	.50021050D-03	.10400750D-04	.10000000D-08	.11504840D-04	.11372090D-03	.79800680D-01
25	.78262360D+00	.34017070D-03	.45604240D-03	.49736110D-03	.12283870D-04	.10000000D-08	.11439300D-04	.11417730D-03	.89803190D-01
26	.88560450D+00	.33781650D-03	.46151160D-03	.49286730D-03	.14411000D-04	.10000000D-08	.11335950D-04	.11474700D-03	.10298090D+00
27	.10067080D+01	.33590100D-03	.46654080D-03	.48688380D-03	.16859440D-04	.10000000D-08	.11198330D-04	.11543860D-03	.12110370D+00
28	.11551360D+01	.33408040D-03	.47291290D-03	.47528090D-03	.19177560D-04	.10000000D-08	.11023460D-04	.11628130D-03	.14847760D+00
29	.13586380D+01	.33190240D-03	.48056170D-03	.46502740D-03	.23625600D-04	.10000000D-08	.10787630D-04	.11739360D-03	.20345180D+00
30	.15531670D+01	.32595900D-03	.48755670D-03	.45558460D-03	.27160580D-04	.10000000D-08	.10570450D-04	.11840310D-03	.19452530D+00
31	.17534290D+01	.32799420D-03	.49454040D-03	.45031120D-03	.30651200D-04	.10000000D-08	.10357160D-04	.11930390D-03	.20026180D+00
32	.19401630D+01	.32610830D-03	.50115020D-03	.44170900D-03	.33913100D-04	.10000000D-08	.10159310D-04	.12028390D-03	.19473400D+00
33	.21428360D+01	.32423940D-03	.50755580D-03	.43350050D-03	.37052410D-04	.10000000D-08	.59705120D-05	.12113330D-03	.15467370D+00
34	.23389150D+01	.32237160D-03	.51394400D-03	.42560120D-03	.40099040D-04	.10000000D-08	.97888280D-05	.12194120D-03	.19607850D+00
35	.25363230D+01	.32051100D-03	.52018370D-03	.41799580D-03	.43056650D-04	.10000000D-08	.96139040D-05	.12270930D-03	.19740660D+00
36	.27369870D+01	.31865850D-03	.52631570D-03	.41067030D-03	.45928660D-04	.10000000D-08	.94454180D-05	.12343930D-03	.15866350D+00
37	.29349160D+01	.31681660D-03	.53235600D-03	.40360870D-03	.48719500D-04	.10000000D-08	.92830000D-05	.12413320D-03	.19992500D+00
38	.31361350D+01	.31498490D-03	.53825660D-03	.39679560D-03	.51433460D-04	.10000000D-08	.91262990D-05	.12479270D-03	.20121520D+00
39	.33386660D+01	.31316470D-03	.54414510D-03	.39021710D-03	.54074520D-04	.10000000D-08	.85749930D-05	.12541960D-03	.20253100D+00
40	.35425290D+01	.31135670D-03	.54990510D-03	.38386020D-03	.56646250D-04	.10000000D-08	.88287850D-05	.12601540D-03	.20386290D+00
41	.37477530D+01	.30956130D-03	.55557570D-03	.37771310D-03	.59152160D-04	.10000000D-08	.86874010D-05	.12658170D-03	.20521450D+00
42	.39543290D+01	.30777810D-03	.56117210D-03	.37176460D-03	.61595330D-04	.10000000D-08	.85505860D-05	.12711970D-03	.20658590D+00
43	.41625070D+01	.30601040D-03	.56668520D-03	.36600450D-03	.63978710D-04	.10000000D-08	.84181030D-05	.12763090D-03	.20797740D+00
44	.43716360D+01	.30425550D-03	.57212190D-03	.36042310D-03	.66305680D-04	.10000000D-08	.82897310D-05	.12811640D-03	.20538540D+00
45	.45825180D+01	.30251470D-03	.57748460D-03	.35501160D-03	.68577030D-04	.10000000D-08	.81652660D-05	.12857740D-03	.21082210D+00
46	.47947050D+01	.30078800D-03	.58277600D-03	.34976150D-03	.70796550D-04	.10000000D-08	.80445150D-05	.12901500D-03	.21227640D+00
47	.50085470D+01	.29907570D-03	.58755870D-03	.34466510D-03	.72967240D-04	.10000000D-08	.79272980D-05	.12943010D-03	.21375260D+00
48	.52238300D+01	.29737770D-03	.59315470D-03	.33971510D-03	.75089990D-04	.10000000D-08	.78134470D-05	.12982380D-03	.21525230D+00
49	.54405760D+01	.29569410D-03	.59824660D-03	.33490460D-03	.77167220D-04	.10000000D-08	.77028050D-05	.13019690D-03	.21677580D+00
50	.56589330D+01	.29402490D-03	.60327620D-03	.33022700D-03	.79200630D-04	.10000000D-08	.75552220D-05	.13055030D-03	.21832440D+00
51	.58787990D+01	.29236580D-03	.60824590D-03	.32567650D-03	.81192750D-04	.10000000D-08	.74905590D-05	.13088490D-03	.21589540D+00
52	.61003010D+01	.29072900D-03	.61315750D-03	.32124720D-03	.83144610D-04	.10000000D-08	.73886850D-05	.13120130D-03	.22150310D+00
53	.63234150D+01	.28910270D-03	.61801310D-03	.31693370D-03	.85058680D-04	.10000000D-08	.72894750D-05	.13150040D-03	.22313400D+00
54	.65482520D+01	.28748940D-03	.62281450D-03	.31273100D-03	.86934650D-04	.10000000D-08	.71528130D-05	.13178270D-03	.22475680D+00
55	.67747240D+01	.28589020D-03	.62756360D-03	.30863420D-03	.88775560D-04	.10000000D-08	.70985870D-05	.13204900D-03	.22649220D+00
56	.70029870D+01	.28430480D-03	.63226220D-03	.30463880D-03	.90583360D-04	.10000000D-08	.70066920D-05	.13229990D-03	.22822240D+00
57	.72329260D+01	.28271160D-03	.63651160D-03	.30074040D-03	.92358680D-04	.10000000D-08	.69170290D-05	.13253580D-03	.22598550D+00
58	.74647120D+01	.28112260D-03	.64151460D-03	.29693490D-03	.94101520D-04	.10000000D-08	.68295030D-05	.13275740D-03	.23179800D+00
59	.76993770D+01	.27962740D-03	.64627190D-03	.29321840D-03	.95814550D-04	.10000000D-08	.67440240D-05	.13296530D-03	.23364440D+00
60	.79339140D+01	.27813190D-03	.65036550D-03	.28958730D-03	.97499520D-04	.10000000D-08	.66605070D-05	.13315990D-03	.23553770D+00
61	.81713930D+01	.27657150D-03	.65505700D-03	.28603780D-03	.99156400D-04	.10000000D-08	.65788690D-05	.13334170D-03	.23747510D+00
62	.84109600D+01	.27536120D-03	.65948810D-03	.28256670D-03	.10078630D-03	.10000000D-08	.64590330D-05	.13351110D-03	.23947220D+00
63	.86523170D+01	.27355560D-03	.66288020D-03	.27517060D-03	.10239140D-03	.10000000D-08	.64209240D-05	.13366850D-03	.24152050D+00
64	.88960310D+01	.27207950D-03	.66823500D-03	.27584670D-03	.10397160D-03	.10000000D-08	.63484750D-05	.13381440D-03	.24361420D+00
65	.91414370D+01	.27060670D-03	.67254330D-03	.27259680D-03	.10552660D-03	.10000000D-08	.62697260D-05	.13394890D-03	.24540600D+00
66	.93397150D+01	.26913650D-03	.67602010D-03	.26541690D-03	.10705580D-03	.10000000D-08	.61565890D-05	.13407250D-03	.24730370D+00
67	.96383270D+01	.26769820D-03	.68105560D-03	.26630370D-03	.10856250D-03	.10000000D-08	.61249850D-05	.13418560D-03	.24931290D+00
68	.98894240D+01	.26626190D-03	.68525570D-03	.26225420D-03	.11004700D-03	.10000000D-08	.60548470D-05	.13428850D-03	.25135450D+00
69	.10142990D+02	.26483560D-03	.68942270D-03	.26026560D-03	.11151040D-03	.10000000D-08	.55861090D-05	.13439150D-03	.25356430D+00
70	.10398810D+02	.26243330D-03	.69355700D-03	.25733520D-03	.11295360D-03	.10000000D-08	.59187090D-05	.13446500D-03	.25582530D+00
71	.10657300D+02	.26231490D-03	.69756210D-03	.25496120D-03	.11437730D-03	.10000000D-08	.58525840D-05	.13453920D-03	.25618520D+00
72	.10917670D+02	.26361890D-03	.70173540D-03	.25163800D-03	.11578380D-03	.10000000D-08	.57876750D-05	.13460450D-03	.26066640D+00
73	.11180340D+02	.25973170D-03	.70579090D-03	.24886630D-03	.11717240D-03	.10000000D-08	.57239220D-05	.13466110D-03	.26326890D+00
74	.11446950D+02	.25785270D-03	.70981900D-03	.24614210D-03	.11854500D-03	.10000000D-08	.56612680D-05	.13470910D-03	.26601070D+00
75	.11715860D+02	.25649110D-03	.71382570D-03	.24346320D-03	.11990240D-03	.10000000D-08	.55965540D-05	.13474900D-03	.26890830D+00
76	.11987840D+02	.25511630D-03	.71781350D-03	.24082710D-03	.12124580D-03	.10000000D-08	.55390230D-05	.13478070D-03	.27198110D+00
77	.12263390D+02	.25375750D-03	.72178510D-03	.23823110D-03	.12257580D-03	.10000000D-08	.54793160D-05	.13480460D-03	.27525240D+00
78	.12541840D+02	.25249370D-03	.72574120D-03	.23567280D-03	.12389410D-03	.10000000D-08	.54204740D-05	.13482670D-03	.27675030D+00
79	.12824350D+02	.25105390D-03	.72969110D-03	.23314930D-03	.12520170D-03	.10000000D-08	.53624340D-05	.13482920D-03	.28250500D+00
80	.13111920D+02	.24970720D-03	.73361220D-03	.23065790D-03	.12649550D-03	.10000000D-08	.53051320D-05	.13483020D-03	.28657070D+00
81	.13401910D+02	.24876670D-03	.73757510D-03	.22819560D-03	.12779000D-03	.10000000D-08	.52484990D-05	.13481910D-03	.29098870D+00
82	.13697740D+02	.24702250D-03	.74151840D-03	.22576030D-03	.12907380D-03	.10000000D-08	.51924860D-05	.13480290D-03	.29583070D+00
83	.14002410D+02	.24566420D-03	.74551660D-03	.22331910D-03	.13036730D-03	.10000000D-08	.51363390D-05	.13477730D-03	.30466550D+00
84	.14311460D+02	.24430350D-03	.74950120D-03	.22091000D-03	.13165200D-03	.10000000D-08	.50809300D-05	.13474560D-03	.30504650D+00
85	.14629200D+02	.24293790D-03	.75354020D-03	.21850310D-03	.13294350D-03	.10000000D-08	.50255010D-05	.13470480D-03	.31774150D+00
86	.14953930D+02	.24156120D-03	.75755570D-03	.21610470D-03	.13423550D-03	.10000000D-08	.49704080D-05	.13465710D-03	.32473330D+00
87	.15000000D+02	.24134930D-03	.75814320D-03	.21576870D-03	.13441650D-03	.10000000D-08	.49626800D-05	.13467080D-03	.46068880D-01

Appendix C

DROP MODEL, SAMPLE INPUT AND OUTPUT

```
C*********************************************************************
C
C     DROP MODEL
C
C     M. F. ALBERT
C
C     THE DROP MODEL SIMULATES THE ABSORPTON OF ONE DROP SUSPENDED IN A
C     GAS CONTAINING MOLECULAR IODINE.  THE DROP MODEL IS A QUASI-
C     STEADY-STATE MODEL THAT CONSIDERS THE MASS TRANSFER INTO THE
C     DROP AND THE IODINE HYDROLYSIS REACTONS WHICH OCCUR IN
C     THE BULK LIQUID OF THE DROP.  A TWO-RESISTANCE MODEL
C     IS USED TO DESCRIBE THE MASS TRANSFER.  A RUNGE-KUTTA-FELHBURG
C     5(4) METHOD IS USED TO NUMERICALLY INTEGRATE THE IODINE
C     HYDROLYSIS REACTIONS.  SUBROUTINES FUNCTN AND ITTER ARE CALLED
C     FROM THIS MAIN PROGRAM.  THIS PROGRAM IS DESIGNED TO RUN ON A
C     PDP-10 COMPUTER BUT SHOULD BE EASILY CONVERTED TO RUN ON ANY
C     FORTRAN COMPUTER.
C
C*********************************************************************
C
      IMPLICIT DOUBLE PRECISION (A-H,K-Z)
      IMPLICIT INTEGER (I-J)
C
      DIMENSION W(8),WOLD(8),K1(7),K2(7),K3(7),R(7),WB(7),
     1     DELTA(7),WES(7),F(7),K4(7),K5(7),K6(7),TOL(7)
C
      READ (58,*)A,B,HMIN,HMAX,IN
      READ (20,*)TEMPG,TEMPL,DIAM
      READ (43,*)CI2G,CHL
      READ (49,*)TOLER
C
10    FORMAT('AT A TEMPERTURE OF THE GAS ',F6.2,' DEGRESS KELVIN'/
     1 'THE VISCOSITY OF THE LIQUID (CP)=',E15.7/
     2 'THE VISCOSITY OF THE GAS (CP) =',E15.7/
     3 'THE PARTITION COEFFICIENT IS =',E15.7/
     4 'THE DENSITY OF THE LIQUID (GMS/CC) =',E15.7/
     5 'THE DENSITY OF THE GAS (GMS/CC) =',E15.7)
11    FORMAT('THE DIFFUSION COEFFICIENT FOR THE GAS (SQ CM/SEC)=',E15.7
     1 /'THE DIFFUSION COEFFICIENT FOR THE LIQUID (SQ CM/SEC)=',E15.7/
     2 'THE GAS-SIDE MASS TRANSFER COEFFICIENT (CM/SEC)='E15.7/
     3 'THE LIQUID-SIDE MASS TRANSFER COEFFICIENT (CM/SEC)=',E15.7/
     4'THE OVERALL LIQUID-SIDE MASS TRANSFER COEFFICIENT (CM/SEC)=',E15.
     57,/, 'THE VOLUME FOR ONE DROP (LITERS)=',E15.7/
     6 'THE SURFACE AREA FOR ONE DROP (SQ CM)=',E15.7/
     7 'THE EXPOSURE TIME FOR THE DROP IS (SEC)=',E15.7/
     8 'THE REYNOLDS NUMBER FOR THE DROP =',E15.7/
     9 'THE TERMINAL VELOCITY OF THE DROP (CM/SEC) =',E15.7)
12    FORMAT('THE CONCENTRATION OF THE GAS IS (MOLES/LITER) :',E15.7,/
     1,'THE INITIAL CONCENTRATION OF THE DROP IS (MOLES/LITER) :')
13    FORMAT('                        I2 = ',E15.7/
     2'                       I- = ',E15.7/
     3'                      HOI = ',E15.7/
     4'                     IO3- = ',E15.7/
     5'                       H+ = ',E15.7/
     6'                      IO- = ',E15.7/
     7'                      I3- = ',E15.7/)
14    FORMAT('THE FINAL CONCENTRATION OF THE DROP IS (MOLES/LITER) :')
15    FORMAT('THE NUMBER OF MOLES OF IODINE (I2) REMOVED IS =',E15.7,/
     1        'THE NUMBER OF GRAMS OF IODINE REMOVES IS =',E15.7,/)
```

```
17    FORMAT('      TIME           MOLES RMD        FALL HGHT        STEP SIZE
     1',/)
19    FORMAT('     N      TIME            I2             I-              HOI
     1      IO3-         H+             IO-            I3-        FALL HGHT'
     2,/)
21    FORMAT('STEP SIZE BELOW STEP MIN',D15.7)
22    FORMAT(I5,9D13.7)
23    FORMAT(4D15.7)
25    FORMAT(I6)
C
      WRITE(50,19)
      WRITE(51,17)
C
      SFA=3.1416D00*(DIAM)**2
      VOLD=(3.1416D00*DIAM**3.D00)/(6.D00*1.0D3)
C
      TEMPG4=TEMPG**4
      TEMPG3=TEMPG**3
      TEMPG2=TEMPG**2
C
      TEMPL4=TEMPL**4
      TEMPL3=TEMPL**3
      TEMPL2=TEMPL**2
C
      VSL1=1.8662866D-8*TEMPL4-2.6333695D-5*TEMPL3+1.3970607D-2*TEMPL2
      VSL2=-3.3074806D00*TEMPL+2.9558666D2
      VISLIQ=VSL1+VSL2
C
      PC1=9.981476D-7*TEMPL4-1.5730121D-3*TEMPL3+9.2785676D-1*TEMPL2
      PC2=-2.4288386D2*TEMPL+2.3824847D4
      PC=PC1+PC2
C
      DNL1=6.0251147D-9*TEMPL3-9.13296040D-6*TEMPL2
      DNL2=3.573572D-3*TEMPL+5.8358882D-1
      DENLIQ=DNL1+DNL2
C
      VSA1=-2.8713293D-15*TEMPG4+1.6909463D-11*TEMPG3-4.015468D-8*TEMPG2
      VSA2=6.5679429D-5*TEMPG+1.9523691D-3
      VISGAS=VSA1+VSA2
C
      TMP=5.178D-3*TEMPG
      OMEGA1=TMP**3*(-6.19047619D-2)+4.657142857D-1*TMP**2
      OMEGA2=TMP*(-1.304238095D00)+2.315428571D00
      OMEGA=OMEGA1+OMEGA2
C
      MLWT=1/2.9D1+1/2.53809D2
C
      DIFGAS=1.858D-3*TEMPG**1.5*MLWT**0.5/(1.0D00*4.4355D00**2*OMEGA)
C
      DIFLIQ=3.91D-8*TEMPL/VISLIQ
C
      DNG1=8.2892055D-16*TEMPG4-4.2656962D-12*TEMPG3+8.0228283D-9*TEMPG2
      DNG2=-6.8325529D-6*TEMPG+2.6129391D-3
      DENGAS=DNG1+DNG2
C
      GSM1=0.83D00*((DENLIQ-DENGAS)/DENGAS)**0.25*9.81D2**0.25
      GSM2=(VISGAS/(1.0D2*DENGAS))**-0.17*DIFGAS**0.67*DIAM**-0.25
      KGI2=GSM1*GSM2
C
      ND1=4.D00*DENGAS*(DENLIQ-DENGAS)*9.81D2*DIAM**3
      ND2=3.0D00*(VISGAS/1.0D2)**2
      ND=ND1/ND2
C
      WW=ALOG10(ND)
```

```
C
      NRE1=(-1.81391D00+1.34671D00*WW-0.12427D00*WW**2+6.344D-3*WW**3)
      NRE=1.0D1**NRE1
C
      TRMVEL=NRE*(VISGAS/1.0D2)/(DIAM*DENGAS)
C
      EXPTM=HEIGHT/TRMVEL
C
      KLI2O=(4.0D00*DIFLIQ*TRMVEL/(3.1415D00*DIAM))**0.5
C
      KLOV=KGI2*KLI2O/(PC*KLI2O+KGI2)
C
      WRITE (22,10) TEMPG,VISLIQ,VISGAS,PC,DENLIQ,DENGAS
      WRITE (22,11) DIFGAS,DIFLIQ,KGI2,KLI2O,KLOV,VOLD,SFA,B,NRE,TRMVEL
C
C     READ IN INITIAL CONDITIONS
C
      DO 20 J=1,7
      READ(58,*) WOLD(J)
20    CONTINUE
C
      TOLD=A
      Q=1.0D-1
      H=5.0D-2
C
C     CALCULATE EQUILIBRIUM CONSTANTS K4, K5 AND K6
C
      RK6=-4.098D00-3245.2D00/TEMPL+2.2363D5/(TEMPL**2)-3.984D7/(TEMPL**
     13)+(13.957D00-1262.3D00/TEMPL+8.5641D5/(TEMPL**2))*DLOG(DENLIQ)
      RK6=10**(RK6)
C
      RK5=10**(2800.48D00+0.7335D00*TEMPL-80670.0D00/TEMPL
     1-1115.1D00*DLOG10(TEMPL))
C
      RK4=DEXP(3727.86D00/TEMPL-11.6326D00+0.0192212D00*TEMPL)
C
      WOLD(8)=RK6/WOLD(5)
C
      WRITE (22,12)CI2G
      WRITE (22,13)WOLD(1),WOLD(2),WOLD(3),WOLD(4),WOLD(5),WOLD(6),
     1              WOLD(7)
C
C     CALCULATE THE MASS TRANSFER
C
      CI2L=WOLD(1)
1     T=TOLD
      WOLD(1)=CI2L
      MOLTR=H*KLOV*(PC*CI2G-WOLD(1))*SFA/1.0D3
      NMOL=WOLD(1)*VOLD
      WOLD(1)=(NMOL+MOLTR)/VOLD
C
C     BEGIN THE RUNGE-KUTTA-FELBBURG ROUTINE
C
C     CALCULATE K'S
C
      DO 30 J=1,IN
       W(J)=WOLD(J)
30    CONTINUE
C
      CALL FUNCTN(W,WOLD,F,IN)
C
      DO 40 J=1,IN
       K1(J)=H*F(J)
40    CONTINUE
C
```

```
      DO 50 J=1,IN
       W(J)=WOLD(J)+K1(J)/4.0D00
50    CONTINUE
C
      CALL FUNCTN(W,WOLD,F,IN)
C
      DO 60 J=1,IN
       K2(J)=H*F(J)
60    CONTINUE
C
      DO 80 J=1,IN
       W(J)=WOLD(J)+3.0D00*K1(J)/3.2D1+9.0D00*K2(J)/3.2D1
80    CONTINUE
C
      CALL FUNCTN(W,WOLD,F,IN)
C
      DO 90 J=1,IN
       K3(J)=H*F(J)
90    CONTINUE
C
      DO 110 J=1,IN
       W(J)=WOLD(J)+1.932D3*K1(J)/2.197D3-7.2D3*K2(J)/2.197D3
     1      +7.296D3*K3(J)/2.197D3
110   CONTINUE
C
      CALL FUNCTN(W,WOLD,F,IN)
C
      DO 120 J=1,IN
       K4(J)=H*F(J)
120   CONTINUE
C
      DO 130 J=1,IN
       W(J)=WOLD(J)+4.39D2*K1(J)/2.16D2-8.0D00*K2(J)+3.68D3*K3(J)/5.13D2
     1      -8.45D2*K4(J)/4.104D3
130   CONTINUE
C
      CALL FUNCTN(W,WOLD,F,IN)
C
      DO 140 J=1,IN
       K5(J)=H*F(J)
140   CONTINUE
C
      DO 150 J=1,IN
       W(J)=WOLD(J)-8.D00*K1(J)/2.7D1+2.D00*K2(J)-3.544D3*K3(J)/2.565D3
     1      +1.859D3*K4(J)/4.104D3-1.1D1*K5(J)/4.0D1
150   CONTINUE
C
      CALL FUNCTN(W,WOLD,F,IN)
C
      DO 160 J=1,IN
       K6(J)=H*F(J)
160   CONTINUE
C
C     DETERMINE THE NEW CONCENTRATION OF ALL IODINE HYDROLYSIS SPECIES
C     AND CHECK ERROR
C
      DO 100 J=1,IN
       WB(J)=WOLD(J)+1.6D1*K1(J)/1.35D2+6.656D3*K3(J)/1.2825D4+
     1       2.8561D4*K4(J)/5.643D4-9.0D00*K5(J)/5.0D1+2.0D00*K6(J)/5.5D1
       R(J)=ABS(K1(J)/3.6D2-1.28D2*K3(J)/4.275D3-2.197D3*K4(J)/7.524D4
     1         +K5(J)/5.0D1+2.0D00*K6(J)/5.5D1)/H
       TOL(J)=ABS(WB(J)*TOLER)
       DELTA(J)=0.98D00*(TOL(J)/R(J))**0.25
100   CONTINUE
C
```

```
      DO 500 J=1,IN
       IF(R(J) .GT. TOL(J))GOTO 900
500   CONTINUE
C
      DO 510 J=1,IN
       WOLD(J)=WB(J)
510   CONTINUE
C
C
C     DETERMINE THE EQUILIBRIUM CONCENTRATION FOR EQUATIONS 23, 24 AND
C     25
C
      BB=-1.0D00-(WOLD(2)+WOLD(1))*RK4
      C=WOLD(2)*WOLD(1)*RK4-WOLD(7)
      D=-BB/(2.0D00*RK4)
      E=((BB**2.0D00-4.0D00*RK4*C)**0.5D00)/(2.0D00*RK4)
      V=D-E
C
      IF(V .LT. 1.0D-18)CALL ITTER(WOLD,RK4,C,V)
C
      WOLD(7)=WOLD(7)+V
      WOLD(1)=WOLD(1)-V
      WOLD(2)=WOLD(2)-V
C
      IF(IN .EQ. 4)GOTO 600
C
      RR=WOLD(6)+WOLD(5)+RK5
      S=-RK5*WOLD(3)+WOLD(6)*WOLD(5)
      M=(-RR+(RR*RR-4.0D00*S)**0.5)/2.0D00
      WOLD(5)=WOLD(5)+M
      GOTO 605
C
600   M=(RK5*WOLD(3)-WOLD(6)*WOLD(5))/(WOLD(5)+RK5)
C
605   WOLD(6)=WOLD(6)+M
      WOLD(3)=WOLD(3)-M
C
      IF(IN .EQ. 4)GOTO 615
C
      U=WOLD(8)*WOLD(5)-RK6
      VV=WOLD(8)+WOLD(5)
      X=(-VV+(VV*VV-4.0D00*U)**0.5)/2.0D00
      WOLD(5)=WOLD(5)+X
      WOLD(8)=WOLD(8)+X
C
615   I=I+1
C
      TOLD=TOLD+H
      FHT=TOLD*TRMVEL
      SUMMOL=SUMMOL+MOLTR
      CI2L=WB(1)
C
      WRITE(51,23)TOLD,SUMMOL,FHT,H
      WRITE(50,22)I,TOLD,WOLD(1),WOLD(2),WOLD(3),WOLD(4),WOLD(5),
     1            WOLD(6),WOLD(7),FHT
C
      DEL=DELTA(1)
C
      IF(IN .EQ. 1)GOTO 905
C
      DO 520 J=2,IN
       IF(DEL .LT. DELTA(J))GOTO 520
       DEL=DELTA(J)
520   CONTINUE
C
      GOTO 905
```

```
C
C     DETERMINE NEW STEP SIZE
C
900   DEL=DELTA(J)
C
905   IF(DEL .GT. Q)GOTO 910
      HNEW=Q*H
      GOTO 1000
C
910   IF(DEL .LT. 4.0)GOTO 920
      HNEW=4.0D00*H
      GOTO 1000
C
920   HNEW=DEL*H
C
C     CHECK NEW STEP SIZE WITH MAX AND MIN STEP SIZE
C
1000  IF (HNEW .LT. HMAX)GOTO 930
      HNEW=HMAX
C
930   IF (HNEW .LT. HMIN)GOTO 1111
      LEFT=B-TOLD-HNEW
C
      IF(LEFT .GT. 0.0)GOTO 5000
      HNEW=B-TOLD
C
5000  H=HNEW
      IF(TOLD .GE. B)GOTO 999
      GOTO 1
C
1111  WRITE(40,21)HNEW
      STOP
C
999   WRITE(23,25)I
      GRMS=253.809D00*SUMMOL
C
      WRITE(22,15)SUMMOL,GRMS
      WRITE(22,14)
      WRITE(22,13)WOLD(1),WOLD(2),WOLD(3),WOLD(4),WOLD(5),WOLD(6),
     1            WOLD(7)
      STOP
      END
```

```
C*************************************************************************
C
C     SUBROUTINE FUNCTN
C
C     THIS SUBROUTINE CONTAINS THE DIFFERENTIAL EQUATIONS (KINETIC RATE
C     EQUATIONS) TO BE INTEGRATED.  THIS SUBROUTINE IS CALLED FROM THE
C     RUNGE-KUTTA-FELHBURG INTEGRATION ROUTINE IN THE KINETIC, DROP,
C     SPRAY AND WALL-SPRAY MODELS.
C
C*************************************************************************
C
      SUBROUTINE FUNCTN (W,WOLD,F,IN)
C
      IMPLICIT DOUBLE PRECISION(A-H,K-Z)
      IMPLICIT INTEGER(I-J)
C
      DIMENSION W(8),WOLD(8),F(7)
C
      IF(IN .EQ. 5)GOTO 5
C
      W(5)=WOLD(5)
5     W(6)=WOLD(6)
C
      RK1=3.0D00
      RKR1=4.4D12
      RK20=2.5D02
      RK21=1.2D02
      RKR2=3.0D08
      RKP3=9.35D-8
C
      R1=RK1*W(1)
      RR1=RKR1*W(2)*W(3)*W(5)
      R20=RK20*W(3)**2.0D00
      R21=RK21*W(3)*W(6)
      RR2=RKR2*W(4)*W(2)**2.0D00*W(5)**2.CD00
      RP3=RKP3*W(5)*W(2)
C
      F(1)=-R1+RR1+5.0D-1*RP3
      F(2)=R1-RR1+2.0D00*(R20+R21)/3.0D00-2.0D00*RR2-RP3
      F(3)=R1-RR1-R20-R21+3.0D00*RR2
      F(4)=(R20+R21)/3.0D00-RR2
C
      IF (IN .EQ. 5)GOTO 10
C
      F(5)=0.0D00
      GOTO 11
C
10    F(5)=R1-RR1+R20+R21-3.0D00*RR2-4.0D00*RP3
C
11    F(6)=0.0D00
      F(7)=0.0D00
C
      RETURN
C
      END
```

```
C*****************************************************************************
C
C     SUBROUTINE ITTER
C
C     THIS SUBROUTINE FINDS THE ROOT TO THE QUADRATIC EQUILIBRIUM
C     EQUATION FOR THE FORMATION REACTION OF TRI-IODIDE, I3- (EQUATION
C     23).  A SECANT METHOD IS THE ROUTINE USED TO FIND THE ROOT.  THIS
C     METHOD IS CALLED WHENEVER THE QUADRATIC FORMULA RESULTS IN LESS
C     THAN APPROXIMATELY THREE SIGNIFICANT FIGURES.  THIS SUBROUTINE
C     IS CALLED BY THE PROGRAMS KINETIC, DROP, SPRAY AND WALL-SPRAY.
C
C*****************************************************************************
C
      SUBROUTINE ITTER(WOLD,RK4,C,V)
C
      IMPLICIT DOUBLE PRECISION (A-H,L-Z)
      IMPLICIT INTEGER (I-K)
C
      DIMENSION WOLD(7),W(7)
C
      P0=1.0D-16
      P1=1.0D-18
C
      Q0=C-RK4*P0*P0-P0*RK4*(WOLD(1)+WOLD(2))-P0
5     Q1=C-RK4*P1*P1-P1*RK4*(WOLD(1)+WOLD(2))-P1
C
      NEW=P1-Q1*(P1-P0)/(Q1-Q0)
C
      CHECK=ABS(NEW-P1)/P1
C
11    IF (CHECK .LT. 1.0D-4) GOTO 10
C
      P0=P1
      Q0=Q1
      P1=NEW
      GOTO 5
C
10    V=NEW
C
      RETURN
C
      END
```

Drop Model sample input:

A = 0.0

B = 15.0

HMIN = 1.0×10^{-10}

HMAX = 1.0×10^{2}

IN = 4

TOLER = 1.0×10^{-4}

TEMPL = 298

TEMPG = 298

DIAM = 0.1

SAD = 0.1

CI2G = 1.0×10^{-5}

WOLD(1) = 0.0

WOLD(2) = 0.0

WOLD(3) = 0.0

WOLD(4) = 0.0

WOLD(5) = 1.0×10^{-9}

WOLD(6) = 0.0

WOLD(7) = 0.0

PRESS = 1.0

```
AT A TEMPERATURE OF THE GAS 298.15 DEGRESS KELVIN
THE VISCOSITY OF THE LIQUID (CP)=  0.8940819E+00
THE VISCOSITY OF THE GAS (CP) =  0.1839068E-01
THE PARTITION COEFFICIENT IS =  0.8634152E+02
THE DENSITY OF THE LIQUID (GMS/CC) =  0.9968763E+00
THE DENSITY OF THE GAS (GMS/CC) =  0.1182484E-02
THE DIFFUSION COEFFICIENT FOR THE GAS (SQ CM/SEC)=  0.8048467E-01
THE DIFFUSION COEFFICIENT FOR THE LIQUID (SQ CM/SEC)=  0.1303870E-04
THE GAS-SIDE MASS TRANSFER COEFFICIENT (CM/SEC)=  0.1128624E+02
THE LIQUID-SIDE MASS TRANSFER COEFFICIENT (CM/SEC)=  0.2558871E+00
THE OVERALL LIQUID-SIDE MASS TRANSFER COEFFICIENT (CM/SEC)=  0.8651918E-01
THE VOLUME FOR ONE DROP (LITERS)=  0.5236000E-06
THE SURFACE AREA FOR ONE DROP (SQ CM)=  0.3141600E-01
THE EXPOSURE TIME FOR THE DROP IS (SEC)=  0.1500000E+02
THE REYNOLDS NUMBER FOR THE DROP =  0.2535929E+03
THE TERMINAL VELOCITY OF THE DROP (CM/SEC) =  0.3944024E+03
THE CONCENTRATION OF THE GAS IS (MOLES/LITER) :  0.1000000E-04
THE INITIAL CONCENTRATION OF THE DROP IS (MOLES/LITER) :
                  I2 =   0.0000000E+00
                  I- =   0.0000000E+00
                 HOI =   0.0000000E+00
                IO3- =   0.0000000E+00
                  H+ =   0.1000000E-08
                 IO- =   0.0000000E+00
                 I3- =   0.0000000E+00
THE NUMBER OF MOLES OF IODINE (I2) REMOVED IS =  0.1269515E-08
THE NUMBER OF GRAMS OF IODINE REMOVES IS =  0.3222144E-06
THE FINAL CONCENTRATION OF THE DROP IS (MOLES/LITER) :
                  I2 =   0.8556520E-03
                  I- =   0.1431969E-02
                 HOI =   0.4027159E-03
                IO3- =   0.3850566E-03
                  H+ =   0.1000000E-08
                 IO- =   0.9273791E-05
                 I3- =   0.9013038E-03
```

FOR50

DAT

File: DSKB:FOR50.DAT[6452,232] Created: 25-Feb-85 10:05:00 <055> Printed: 25-Feb-85 10:06:25
QUEUE Switches: /FILE:FORT /COPIES:1 /SPACING:1 /LIMIT:187

#	TIME	I2	I-	HOI	IO3-	H+	IO-	I3-	FALL HGHT
1	.1339196D-01	.5756464D-04	.2267530D-05	.2310411D-05	.2099250D-11	.1000000D-08	.5320442D-07	.9609611D-07	.5281021D+01
2	.2654436D-01	.1079178D-03	.6226959D-05	.6570255D-05	.2619317D-10	.1000000D-08	.1513006D-06	.4947277D-06	.1046916D+02
3	.4448333D-01	.1660106D-03	.1430235D-04	.1570852D-04	.2287861D-09	.1000000D-08	.3617377D-06	.1769054D-05	.1754433D+02
4	.6880054D-01	.2356272D-03	.2904655D-04	.3331045D-04	.1541621D-08	.1000000D-08	.7670770D-06	.5038682D-05	.2713510D+02
5	.1009615D+00	.3049691D-03	.5336648D-04	.6383673D-04	.8298961D-08	.1000000D-08	.1470040D-05	.1198178D-04	.3981946D+02
6	.1420913D+00	.3686557D-03	.8970257D-04	.1113043D-03	.3618200D-07	.1000000D-08	.2563128D-05	.2434573D-04	.5604113D+02
7	.1925709D+00	.4213377D-03	.1386532D-03	.1769458D-03	.1282966D-06	.1000000D-08	.4074729D-05	.4300879D-04	.7595042D+02
8	.2517266D+00	.4628050D-03	.1976747D-03	.2572433D-03	.3717988D-06	.1000000D-08	.5923830D-05	.6735143D-04	.9928158D+02
9	.3180686D+00	.4973474D-03	.2613903D-03	.3446914D-03	.8937718D-06	.1000000D-08	.7937596D-05	.9570758D-04	.1254470D+03
10	.3901131D+00	.5299311D-03	.3239698D-03	.4312752D-03	.1831110D-05	.1000000D-08	.9931457D-05	.1263924D-03	.1538615D+03
11	.4670652D+00	.5634243D-03	.3814236D-03	.5113483D-03	.3302441D-05	.1000000D-08	.1177539D-04	.1582123D-03	.1842116D+03
12	.5488670D+00	.5984010D-03	.4320693D-03	.5820137D-03	.5399805D-05	.1000000D-08	.1340268D-04	.1903462D-03	.2164744D+03
13	.6359132D+00	.6340421D-03	.4758404D-03	.6422127D-03	.8190598D-05	.1000000D-08	.1470895D-04	.2221142D-03	.2500057D+03
14	.7266270D+00	.6687035D-03	.5124994D-03	.6907495D-03	.1162943D-04	.1000000D-08	.1590666D-04	.2523039D-03	.2865834D+03
15	.8178477D+00	.7002477D-03	.5423152D-03	.7278734D-03	.1653314D-04	.1000000D-08	.1675235D-04	.2795763D-03	.3225610D+03
16	.9110385D+00	.7275046D-03	.5677557D-03	.7550383D-03	.1988294D-04	.1000000D-08	.1738711D-04	.3040845D-03	.3593157D+03
17	.1006670D+01	.7507019D-03	.5899463D-03	.7749907D-03	.2463070D-04	.1000000D-08	.1784658D-04	.3260446D-03	.3970331D+03
18	.1105313D+01	.7701868D-03	.6097398D-03	.7886117D-03	.2973964D-04	.1000000D-08	.1816025D-04	.3457304D-03	.4359381D+03
19	.1207448D+01	.7863689D-03	.6277411D-03	.7969327D-03	.3517412D-04	.1000000D-08	.1835186D-04	.3634140D-03	.4762263D+03
20	.1313522D+01	.7996374D-03	.6444069D-03	.8008181D-03	.4090128D-04	.1000000D-08	.1844133D-04	.3793589D-03	.5180561D+03
21	.1423938D+01	.8103872D-03	.6600869D-03	.8010060D-03	.4688975D-04	.1000000D-08	.1844566D-04	.3938136D-03	.5616046D+03
22	.1539049D+01	.8189718D-03	.6750536D-03	.7981390D-03	.5310883D-04	.1000000D-08	.1837964D-04	.4070092D-03	.6070044D+03
23	.1659132D+01	.8257217D-03	.6895191D-03	.7927831D-03	.5952738D-04	.1000000D-08	.1825631D-04	.4191572D-03	.6543654D+03
24	.1784367D+01	.8309392D-03	.7036463D-03	.7854441D-03	.6611257D-04	.1000000D-08	.1808730D-04	.4304479D-03	.7037585D+03
25	.1914804D+01	.8348909D-03	.7175551D-03	.7765739D-03	.7282928D-04	.1000000D-08	.1788304D-04	.4410482D-03	.7552012D+03

26	.2050151D+01	.8378530D-03	.7313059D-03	.7665929D-03	.7963009D-04	.1000000D-08	.1765319D-04	.4510907D-03	.8085844D+03
27	.2189309D+01	.8400397D-03	.7448618D-03	.7559293D-03	.8643527D-04	.1000000D-08	.1740763D-04	.4606515D-03	.8634685D+03
28	.2331926D+01	.8416210D-03	.7582705D-03	.7448874D-03	.9321136D-04	.1000000D-08	.1715336D-04	.4698267D-03	.9197173D+03
29	.2477379D+01	.8427627D-03	.7715241D-03	.7327241D-03	.9991839D-04	.1000000D-08	.1689629D-04	.4786876D-03	.9770841D+03
30	.2625090D+01	.8435903D-03	.7846118D-03	.7226328D-03	.1065257D-03	.1000000D-08	.1664088D-04	.4872873D-03	.1035341D+04
31	.2774507D+01	.8442029D-03	.7975254D-03	.7117540D-03	.1130089D-03	.1000000D-08	.1639036D-04	.4956635D-03	.1094272D+04
32	.2925168D+01	.8446627D-03	.8102432D-03	.7011804D-03	.1193518D-03	.1000000D-08	.1614687D-04	.5038432D-03	.1153693D+04
33	.3076700D+01	.8450252D-03	.8227586D-03	.6909675D-03	.1255450D-03	.1000000D-08	.1591168D-04	.5118457D-03	.1213458D+04
34	.3228824D+01	.8453232D-03	.8350659D-03	.6811426D-03	.1315846D-03	.1000000D-08	.1568543D-04	.5196854D-03	.1273456D+04
35	.3381335D+01	.8455786D-03	.8471636D-03	.6717141D-03	.1374709D-03	.1000000D-08	.1546831D-04	.5273734D-03	.1333607D+04
36	.3534091D+01	.8458063D-03	.8590528D-03	.6626773D-03	.1432068D-03	.1000000D-08	.1526021D-04	.5349186D-03	.1393854D+04
37	.3686991D+01	.8460159D-03	.8707368D-03	.6540202D-03	.1487960D-03	.1000000D-08	.1506085D-04	.5423284D-03	.1454158D+04
38	.3839968D+01	.8462137D-03	.8822200D-03	.6457261D-03	.1542466D-03	.1000000D-08	.1486986D-04	.5496091D-03	.1514493D+04
39	.3992976D+01	.8464033D-03	.8935080D-03	.6377766D-03	.1595621D-03	.1000000D-08	.1468680D-04	.5567661D-03	.1574839D+04
40	.4145984D+01	.8465874D-03	.9046065D-03	.6301525D-03	.1647494D-03	.1000000D-08	.1451123D-04	.5638044D-03	.1635186D+04
41	.4298971D+01	.8467672D-03	.9155216D-03	.6228344D-03	.1698145D-03	.1000000D-08	.1434271D-04	.5707285D-03	.1695524D+04
42	.4451922D+01	.8469437D-03	.9262591D-03	.6158051D-03	.1747631D-03	.1000000D-08	.1418083D-04	.5775426D-03	.1755849D+04
43	.4604829D+01	.8471173D-03	.9368250D-03	.6090463D-03	.1796008D-03	.1000000D-08	.1402519D-04	.5842503D-03	.1816155D+04
44	.4757683D+01	.8472882D-03	.9472250D-03	.6025421D-03	.1843326D-03	.1000000D-08	.1387541D-04	.5908555D-03	.1876442D+04
45	.4910481D+01	.8474565D-03	.9574646D-03	.5962773D-03	.1889635D-03	.1000000D-08	.1373115D-04	.5973613D-03	.1936705D+04
46	.5063219D+01	.8476224D-03	.9675490D-03	.5902380D-03	.1934980D-03	.1000000D-08	.1359207D-04	.6037712D-03	.1996945D+04
47	.5215893D+01	.8477851D-03	.9774834D-03	.5844112D-03	.1979405D-03	.1000000D-08	.1345789D-04	.6100879D-03	.2057161D+04
48	.5368503D+01	.8479464D-03	.9872726D-03	.5787847D-03	.2022946D-03	.1000000D-08	.1332832D-04	.6163146D-03	.2117350D+04
49	.5521045D+01	.8481046D-03	.9969211D-03	.5733476D-03	.2065645D-03	.1000000D-08	.1320312D-04	.6224539D-03	.2177513D+04
50	.5673518D+01	.8482601D-03	.1006434D-02	.5680894D-03	.2107541D-03	.1000000D-08	.1308203D-04	.6285084D-03	.2237649D+04
51	.5825922D+01	.8484130D-03	.1015814D-02	.5630007D-03	.2148652D-03	.1000000D-08	.1296485D-04	.6344807D-03	.2297757[illegible]
52	.5978254D+01	.8485633D-03	.1025066D-02	.5580724D-03	.2189031D-03	.1000000D-08	.1285136D-04	.6403732D-03	.2357837D+04
53	.6130513D+01	.8487109D-03	.1034195D-02	.5532965D-03	.2228690D-03	.1000000D-08	.1274138D-04	.6461881D-03	.2417889D+04
54	.6282699D+01	.8488558D-03	.1043202D-02	.5486651D-03	.2267660D-03	.1000000D-08	.1263473D-04	.6519277D-03	.2477911D+04
55	.6434810D+01	.8489981D-03	.1052093D-02	.5441713D-03	.2305969D-03	.1000000D-08	.1253124D-04	.6575940D-03	.2537904D+04
56	.6586846D+01	.8491378D-03	.1060870D-02	.5398082D-03	.2343641D-03	.1000000D-08	.1243077D-04	.6631892D-03	.2597864D+04
57	.6738805D+01	.8492749D-03	.1069537D-02	.5355698D-03	.2380698D-03	.1000000D-08	.1233317D-04	.6687150D-03	.2657800D+04
58	.6890686D+01	.8494094D-03	.1078096D-02	.5314501D-03	.2417163D-03	.1000000D-08	.1223830D-04	.6741735D-03	.2717703D+04
59	.7042489D+01	.8495414D-03	.1086551D-02	.5274437D-03	.2453056D-03	.1000000D-08	.1214604D-04	.6795663D-03	.2777574D+04
60	.7194213D+01	.8496709D-03	.1094905D-02	.5235456D-03	.2488396D-03	.1000000D-08	.1205627D-04	.6848952D-03	.2837415D+04
61	.7345858D+01	.8497980D-03	.1103159D-02	.5197509D-03	.2523203D-03	.1000000D-08	.1196889D-04	.6901618D-03	.2897224D+04
62	.7497422D+01	.8499227D-03	.1111318D-02	.5160551D-03	.2557493D-03	.1000000D-08	.1188378D-04	.6953678D-03	.2957001D+04
63	.7648905D+01	.8500450D-03	.1119382D-02	.5124540D-03	.2591283D-03	.1000000D-08	.1180085D-04	.7005146D-03	.3016746D+04
64	.7800306D+01	.8501650D-03	.1127355D-02	.5089437D-03	.2624590D-03	.1000000D-08	.1172007D-04	.7056037D-03	.3076459D+04
65	.7951625D+01	.8502828D-03	.1135239D-02	.5055203D-03	.2657428D-03	.1000000D-08	.1164118D-04	.7106366D-03	.3136139D+04
66	.8102861D+01	.8503983D-03	.1143036D-02	.5021803D-03	.2689812D-03	.1000000D-08	.1156427D-04	.7156146D-03	.3195787D+04
67	.8254014D+01	.8505117D-03	.1150748D-02	.4989205D-03	.2721755D-03	.1000000D-08	.1148920D-04	.7205390D-03	.3255403D+04
68	.8405083D+01	.8506229D-03	.1158378D-02	.4957375D-03	.2753271D-03	.1000000D-08	.1141590D-04	.7254111D-03	.3314985D+04
69	.8556069D+01	.8507321D-03	.1165926D-02	.4926285D-03	.2784371D-03	.1000000D-08	.1134431D-04	.7302321D-03	.3374534D+04
70	.8706[illegible]D+01	.8508392D-03	.1173396D-02	.4895907D-03	.2815065D-03	.1000000D-08	.1127435D-04	.7350032D-03	.3434049D+04
71	.8857786D+01	.8509444D-03	.1180789D-02	.4866212D-03	.2845376D-03	.1000000D-08	.1120597D-04	.7397256D-03	.3493532D+04
72	.9008518D+01	.8510477D-03	.1188107D-02	.4837177D-03	.2875302D-03	.1000000D-08	.1113911D-04	.7444003D-03	.3552981D+04
73	.9159164D+01	.8511491D-03	.1195352D-02	.4808776D-03	.2904857D-03	.1000000D-08	.1107371D-04	.7490284D-03	.3612396D+04
74	.9309725D+01	.8512486D-03	.1202524D-02	.4780987D-03	.2934053D-03	.1000000D-08	.1100971D-04	.7536109D-03	.3671777D+04
75	.9460230D+01	.8513463D-03	.1209626D-02	.4753788D-03	.2962896D-03	.1000000D-08	.1094708D-04	.7581488D-03	.3731125D+04
76	.9610589D+01	.8514423D-03	.1216660D-02	.4727159D-03	.2991402D-03	.1000000D-08	.1088576D-04	.7626431D-03	.3790439D+04
77	.9760892D+01	.8515366D-03	.1223626D-02	.4701080D-03	.3019574D-03	.1000000D-08	.1082570D-04	.7670947D-03	.3849719D+04
78	.9911109D+01	.8516292D-03	.1230527D-02	.4675532D-03	.3047422D-03	.1000000D-08	.1076687D-04	.7715046D-03	.3908965D+04
79	.1006124D+02	.8517202D-03	.1237363D-02	.4650496D-03	.3074955D-03	.1000000D-08	.1070922D-04	.7758735D-03	.3968177D+04
80	.1021128D+02	.8518096D-03	.1244135D-02	.4625957D-03	.3102179D-03	.1000000D-08	.1065271D-04	.7802024D-03	.4027355D+04
81	.1036124D+02	.8518975D-03	.1250847D-02	.4601898D-03	.3129104D-03	.1000000D-08	.1059731D-04	.7844920D-03	.4086499D+04
82	.1051112D+02	.8519838D-03	.1257498D-02	.4578303D-03	.3155736D-03	.1000000D-08	.1054297D-04	.7887431D-03	.4145609D+04
83	.1066090D+02	.8520687D-03	.1264090D-02	.4555157D-03	.3182081D-03	.1000000D-08	.1048967D-04	.7929566D-03	.4204684D+04
84	.1081060D+02	.8521521D-03	.1270623D-02	.4532447D-03	.3208148D-03	.1000000D-08	.1043737D-04	.7971331D-03	.4263726D+04
85	.1096021D+02	.8522341D-03	.1277100D-02	.4510158D-03	.3233943D-03	.1000000D-08	.1038605D-04	.8012734D-03	.4322734D+04
86	.1110974D+02	.8523148D-03	.1283521D-02	.4488278D-03	.3259471D-03	.1000000D-08	.1033566D-04	.8053782D-03	.4381707D+04
87	.1125918D+02	.8523941D-03	.1289887D-02	.4466794D-03	.3284739D-03	.1000000D-08	.1028619D-04	.8094481D-03	.4440647D+04
88	.1140853D+02	.8524721D-03	.1296199D-02	.4445695D-03	.3309752D-03	.1000000D-08	.1023760D-04	.8134839D-03	.4499552D+04
89	.1155780D+02	.8525488D-03	.1302459D-02	.4424968D-03	.3334517D-03	.1000000D-08	.1018987D-04	.8174861D-03	.4558424D+04
90	.1170698D+02	.8526243D-03	.1308668D-02	.4404604D-03	.3359039D-03	.1000000D-08	.1014297D-04	.8214554D-03	.4617262D+C8
91	.1185608D+02	.8526986D-03	.1314825D-02	.4384591D-03	.3383323D-03	.1000000D-08	.1009689D-04	.8253924D-03	.4676065D+04
92	.1200509D+02	.8527716D-03	.1320933D-02	.4364919D-03	.3407374D-03	.1000000D-08	.1005159D-04	.8292978D-03	.4734835D+04
93	.1215401D+02	.8528436D-03	.1326992D-02	.4345579D-03	.3431198D-03	.1000000D-08	.1000705D-04	.8331719D-03	.4793571D+04
94	.1230285D+02	.8529144D-03	.1333003D-02	.4326561D-03	.3454798D-03	.1000000D-08	.9963257D-05	.8370155D-03	.4852274D+04
95	.1245160D+02	.8529840D-03	.1338967D-02	.4307857D-03	.3478180D-03	.1000000D-08	.9920185D-05	.8408291D-03	.4910942D+04
96	.1260027D+02	.8530526D-03	.1344885D-02	.4289458D-03	.3501348D-03	.1000000D-08	.9877815D-05	.8446131D-03	.4969577D+04
97	.1274885D+02	.8531202D-03	.1350757D-02	.4271355D-03	.3524307D-03	.1000000D-08	.9836128D-05	.8483681D-03	.5028178D+04
98	.1289735D+02	.8531867D-03	.1356584D-02	.4253541D-03	.3547060D-03	.1000000D-08	.9795105D-05	.8520947D-03	.5086746D+04
99	.1304577D+02	.8532522D-03	.1362368D-02	.4236008D-03	.3569612D-03	.1000000D-08	.9754729D-05	.8557932D-03	.5145281D+04
100	.1319409D+02	.8533167D-03	.1368109D-02	.4218748D-03	.3591966D-03	.1000000D-08	.9714983D-05	.8594642D-03	.5203782D+04
101	.1334234D+02	.8533803D-03	.1373807D-02	.4201755D-03	.3614127D-03	.1000000D-08	.9675851D-05	.8631081D-03	.5262249D+04
102	.1349050D+02	.8534429D-03	.1379463D-02	.4185021D-03	.3636099D-03	.1000000D-08	.9637317D-05	.8667254D-03	.5320684D+04
103	.1363857D+02	.8535045D-03	.1385079D-02	.4168540D-03	.3657884D-03	.1000000D-08	.9599364D-05	.8703166D-03	.5379085D+04
104	.1378656D+02	.8535653D-03	.1390654D-02	.4152306D-03	.3679486D-03	.1000000D-08	.9561980D-05	.8738819D-03	.5437454D+04
105	.1393447D+02	.8536252D-03	.1396189D-02	.4136312D-03	.3700910D-03	.1000000D-08	.9525149D-05	.8774219D-03	.5495789D+04
106	.1408230D+02	.8536843D-03	.1401686D-02	.4120553D-03	.3722157D-03	.1000000D-08	.9488858D-05	.8809370D-03	.5554091D+04
107	.1423004D+02	.8537425D-03	.1407144D-02	.4105022D-03	.3743232D-03	.1000000D-08	.9453098D-05	.8844276D-03	.5612361D+04
108	.1437770D+02	.8537998D-03	.1412564D-02	.4089715D-03	.3764137D-03	.1000000D-08	.9417844D-05	.8878940D-03	.5670558D+04
109	.1452527D+02	.8538564D-03	.1417947D-02	.4074625D-03	.3784876D-03	.1000000D-08	.9383095D-05	.8913366D-03	.5728802D+04
110	.1467277D+02	.8539121D-03	.1423293D-02	.4059748D-03	.3805451D-03	.1000000D-08	.9348835D-05	.8947558D-03	.5786974D+04
111	.1482018D+02	.8539671D-03	.1428604D-02	.4045078D-03	.3825865D-03	.1000000D-08	.9315054D-05	.8981520D-03	.5845114D+04
112	.1496751D+02	.8540214D-03	.1433878D-02	.4030611D-03	.3846122D-03	.1000000D-08	.9281740D-05	.9015255D-03	.5903221D+04
113	.1500000D+02	.8556520D-03	.1433969D-02	.4027159D-03	.3850566D-03	.1000000D-08	.9273791D-05	.9033038D-03	.5916035D+04

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FFFFFFFFFFFF      OOO         OOO    RRRRRRRRRRRR               555           111
FFFFFFFFFFFF      OOO         OOO    RRRRRRRRRRRR               555           111
FFFFFFFFFFFF      OOO         OOO    RRRRRRRRRRRR               555           111
FFF               OOO         OOO    RRR   RRR                     555        111
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FFF                  OOOOOOOOO       RRR         RRR      555555555        111111111
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File: DSKB:FOR51.DAT[6452,232] Created: 25-Feb-85 10:04:00 <055> Printed: 25-Feb-85 10:06:28
QUEUE Switches: /FILE:FORT /COPIES:1 /SPACING:1 /LIMIT:105

TIME	MOLES PMD	FALL HGHT	STEP SIZE
0.1339196D-01	0.3142876D-10	0.5281821D+01	0.1339196D-01
0.2654436D-01	0.6023395D-1(	0.1046916D+02	0.1315239D-01
0.4448333D-01	0.9705233D-10	0.1754[illegible]33D+02	0.1793897D-01
0.6880054D-01	0.1429318D-09	0.27135[illegible]0D+02	0.2431721D-01
0.1009615D+00	0.1975249D-09	0.398194[illegible]D+02	0.3216098D-01
0.1420913D+00	0.2591797D-09	0.560411[illegible]+02	0.4112974D-01
0.1925709D+00	0.3253683D-09	0.7595042D+02	0.5047965D-01
0.2517266D+00	0.3934491D-09	0.9928158D+02	0.5915573D-01
0.3180686D+00	0.4612989D-09	0.1254470D+03	0.6634197D-01
0.3901131D+00	0.5274306D-09	0.1538615D+03	0.7204445D-01
0.4670652D+00	0.5907649D-09	0.1842116D+03	0.7695215D-01
0.5408670D+00	0.6503912D-09	0.2164784D+03	0.8180173D-01
0.6359132D+00	0.7054900D-09	0.2508057D+03	0.8704626D-01
0.7266270D+00	0.7542131D-09	0.2865834D+03	0.9071384D-01
0.8178477D+00	0.7950056D-09	0.3225610D+03	0.9122061D-01
0.9110385D+00	0.8294279D-09	0.3593157D+03	0.9319082D-01
0.1006670D+01	0.8583854D-09	0.3970331D+03	0.9563170D-01
0.1105313D+01	0.8827181D-09	0.4359381D+03	0.9864299D-01
0.1207448D+01	0.9031344D-09	0.4762203D+03	0.1021347D+00
0.1313522D+01	0.9202508D-09	0.5180561D+03	0.1060738D+00
0.1423938D+01	0.9346065D-09	0.5616046D+03	0.1104164D+00
0.1539049D+01	0.9466754D-09	0.6070044D+03	0.1151104D+00
0.1659132D+01	0.9568745D-09	0.6543654D+03	0.1200831D+00
0.1784367D+01	0.9655702D-09	0.7037585D+03	0.1252352D+00
0.1914804D+01	0.9730812D-09	0.7552032D+03	0.1304371D+00
0.2050151D+01	0.9796723D-09	0.8085844D+03	0.1353470D+00
0.2189309D+01	0.9855425D-09	0.8634685D+03	0.1391578D+00
0.2331926D+01	0.99089[illegible]8D-09	0.9197173D+03	0.1426176D+00
0.2477379D+01	0.9958867D-09	0.9770841D+03	0.1454527D+00

0.2625090D+01	0.1000621D-08	0.1035341D+04	0.1477104D+00
0.2774507D+01	0.1005180D-08	0.1094272D+04	0.1494178D+00
0.2925168D+01	0.1009618D-08	0.1153693D+04	0.1506606D+00
0.3076700D+01	0.1013973D-08	0.1213458D+04	0.1515322D+00
0.3228824D+01	0.1018263D-08	0.1273456D+04	0.1521237D+00
0.3381335D+01	0.1022518D-08	0.1333607D+04	0.1525115D+00
0.3534091D+01	0.1026732D-08	0.1393854D+04	0.1527556D+00
0.3686991D+01	0.1030915D-08	0.1454158D+04	0.1529003D+00
0.3839968D+01	0.1035068D-08	0.1514433D+04	0.1529771D+00
0.3992976D+01	0.1039194D-08	0.1574839D+04	0.1530080D+00
0.4145984D+01	0.1043293D-08	0.1635186D+04	0.1530078D+00
0.4298971D+01	0.1047364D-08	0.1695524D+04	0.1529867D+00
0.4451922D+01	0.1051406D-08	0.1755849D+04	0.1529514D+00
0.4604829D+01	0.1055420D-08	0.1816155D+04	0.1529064D+00
0.4757683D+01	0.1059404D-08	0.1876442D+04	0.1528546D+00
0.4910481D+01	0.1063359D-08	0.1936705D+04	0.1527979D+00
0.5063219D+01	0.1067283D-08	0.1996945D+04	0.1527376D+00
0.5215893D+01	0.1071177D-08	0.2057161D+04	0.1526745D+00
0.5368503D+01	0.1075040D-08	0.2117350D+04	0.1526093D+00
0.5521045D+01	0.1078872D-08	0.2177513D+04	0.1525422D+00
0.5673518D+01	0.1082673D-08	0.2237649D+04	0.1524735D+00
0.5825922D+01	0.1086443D-08	0.2297757D+04	0.1524034D+00
0.5978254D+01	0.1090182D-08	0.2357837D+04	0.1523321D+00
0.6130513D+01	0.1093890D-08	0.2417889D+04	0.1522595D+00
0.6282699D+01	0.1097567D-08	0.2477911D+04	0.1521959D+00
0.6434810D+01	0.1101213D-08	0.2537904D+04	0.1521112D+00
0.6586846D+01	0.1104830D-08	0.2597868D+04	0.1520355D+00
0.6718805D+01	0.1108416D-08	0.2657800D+04	0.1519589D+00
0.6890686D+01	0.1111972D-08	0.2717703D+04	0.1518814D+00
0.7042489D+01	0.1115499D-08	0.2777574D+04	0.1518032D+00
0.7194213D+01	0.1118996D-08	0.2837415D+04	0.1517241D+00
0.7345858D+01	0.1122465D-08	0.2897224D+04	0.1516444D+00
0.7497422D+01	0.1125905D-08	0.2957001D+04	0.1515639D+00
0.7648905D+01	0.1129317D-08	0.3016746D+04	0.1514828D+00
0.7800306D+01	0.1132701D-08	0.3076459D+04	0.1514012D+00
0.7951625D+01	0.1136058D-08	0.3136139D+04	0.1513189D+00
0.8102861D+01	0.1139387D-08	0.3195787D+04	0.1512362D+00
0.8254014D+01	0.1142690D-08	0.3255403D+04	0.1511530D+00
0.8405083D+01	0.1145966D-08	0.3314985D+04	0.1510694D+00
0.8556069D+01	0.1149217D-08	0.3374534D+04	0.1509854D+00
0.8706970D+01	0.1152442D-08	0.3434049D+04	0.1509011D+00
0.8057786D+01	0.1155641D-08	0.3493532D+04	0.1508164D+00
0.9008518D+01	0.1158816D-08	0.3552981D+04	0.1507314D+00
0.9159164D+01	0.1161966D-08	0.3612396D+04	0.1506462D+00
0.9309725D+01	0.1165091D-08	0.3671777D+04	0.1505607D+00
0.9460200D+01	0.1168193D-08	0.3731125D+04	0.1504751D+00
0.9610589D+01	0.1171272D-08	0.3790439D+04	0.1503892D+00
0.9760892D+01	0.1174327D-08	0.3849719D+04	0.1503033D+00
0.9911109D+01	0.1177359D-08	0.3908965D+04	0.1502172D+00
0.1006124D+02	0.1180369D-08	0.3968177D+04	0.1501310D+00
0.1021128D+02	0.1183357D-08	0.4027355D+04	0.1500447D+00
0.1036124D+02	0.1186323D-08	0.4086499D+04	0.1499584D+00
0.1051112D+02	0.1189268D-08	0.4145609D+04	0.1498720D+00
0.1066090D+02	0.1192191D-08	0.4204684D+04	0.1497856D+00
0.1081060D+02	0.1195094D-08	0.4263726D+04	0.1496992D+00
0.1096021D+02	0.1197975D-08	0.4322734D+04	0.1496128D+00
0.1110974D+02	0.1200837D-08	0.4381707D+04	0.1495265D+00
0.1125918D+02	0.1203679D-08	0.4440647D+04	0.1494402D+00
0.1140853D+02	0.1206500D-08	0.4499552D+04	0.1493539D+00
0.1155780D+02	0.1209303D-08	0.4558424D+04	0.1492678D+00
0.1170698D+02	0.1212086D-08	0.4617262D+04	0.1491817D+00
0.1185608D+02	0.1214851D-08	0.4676065D+04	0.1490957D+00
0.1200509D+02	0.1217597D-08	0.4734835D+04	0.1490099D+00
0.1215401D+02	0.1220324D-08	0.4793571D+04	0.1489242D+00
0.1230285D+02	0.1223034D-08	0.4852274D+04	0.1488386D+00
0.1245160D+02	0.1225725D-08	0.4910942D+04	0.1487531D+00
0.1260027D+02	0.1228399D-08	0.4969577D+04	0.1486678D+00
3.1274885D+02	0.1231056D-08	0.5028178D+04	0.1485827D+00
0.1289735D+02	0.1233696D-08	0.5086746D+04	0.1484977D+00
0.1304577D+02	0.1236319D-08	0.5145281D+04	0.1484129D+00
0.1319409D+02	0.1238925D-08	0.5203782D+04	0.1483283D+00
0.1334234D+02	0.1241515D-08	0.5262249D+04	0.1482439D+00
0.1349050D+02	0.1244089D-08	0.5320684D+04	0.1481597D+00
0.1363857D+02	0.1246647D-08	0.5379085D+04	0.1480756D+00
0.1378656D+02	0.1249189D-08	0.5437454D+04	0.1479918D+00
0.1393447D+02	0.1251715D-08	0.5495789D+04	0.1479082D+00
0.1408230D+02	0.1254227D-08	0.5554091D+04	0.1478249D+00
0.1423004D+02	0.1256723D-08	0.5612361D+04	0.1477417D+00
0.1437770D+02	0.1259204D-08	0.5670598D+04	0.1476588D+00
0.1452527D+02	0.1261670D-08	0.5728802D+04	0.1475761D+00
0.1467277D+02	0.1264122D-08	0.5786974D+04	0.1474937D+00
0.1482018D+02	0.1266560D-08	0.5845114D+04	0.1474115D+00
0.1496751D+02	0.1268984D-08	0.5903221D+04	0.1473295D+00
0.1500000D+02	0.1269515D-08	0.5916035D+04	0.3249097D-01

Appendix D

SPRAY MODEL, SAMPLE INPUT AND OUTPUT

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C***********************************************************************
C
C      SPRAY MODEL
C      M. F. ALBERT
C
C      THE SPRAY MODEL SIMULATES THE REMOVAL OF MOLECULAR IODINE, I2,
C      FROM A GAS PHASE BY A SPRAY SYSTEM.  THIS MODEL IS QUASI-STEADY-
C      STATE MODEL THAT DETERMINES THE ABSORPTION OF GASEOUS IODINE
C      INTO THE SPRAY DROPLETS AND THEN REACTS THE IODINE SPECIES
C      ACCORDING TO THE IODINE HYDROLYSIS REACTIONS.  A TWO-RESISTANCE
C      MODEL IS USED TO DETERMINE THE MASS TRANSFER AND A RUNGE-KUTTA-
C      FELHBURG 5(4) NUMERICAL INTEGRATION ROUTINE IS USED TO INTEGRATE
C      THE IODINE HYDROLYSIS REACTIONS.  THIS MAIN PROGRAM CALLS THE
C      SUBROUTINES ITTER AND FUNCTN.  THIS PROGRAM IS DESIGNED TO RUN
C      ON A PDP-10 COMPUTER BUT SHOULD BE EASILY CONVERTED TO RUN ON
C      ANY FORTRAN MACHINE.
C
C      THIS PROGRAM IS VALID FOR GAS PHASE TEMPERATURES OF 273K TO 1500K
C      AND LIQUID PHASE TEMPERATURES OF 273K TO 385K.  THIS PROGRAM
C      SHOULD NOT BE USED OUTSIDE THESE TEMPERATURE RANGES BECAUSE THE
C      INTERNALLY DETERMINED PHYSICAL PROPERTIES MAY BE INCORRECT.
C      FILE FOR22.DAT PROVIDES A SUMMARY OF THE CALCULATIONS OF THIS
C      PROGRAM AND THE INTERNALLY CALCULATED RESULTS CAN BE CHECKED.
C      OTHER TEMPERATURES CAN BE USED IF ONE INCORPORATES NEW
C      CORRELATIONS FOR THE PHYSICAL PROPERTIES.
C
C***********************************************************************
C
      IMPLICIT DOUBLE PRECISION (A-H,K-Z)
      IMPLICIT INTEGER (I-J)
C
      DIMENSION W(8),WOLD(8),K1(7),K2(7),K3(7),R(7),WB(7),
     1      DELTA(7),WES(7),F(7),K4(7),K5(7),K6(7),TOL(7),
     2      CCB(7),CC(7),CONPOL(8)
C
      READ (58,*)A,HMIN,HMAX,IN
      READ (49,*)TOLER
      READ (31,*)TEMPG,TEMPL,PRESS,DIAM,SAD,CI2SP,CISP
      READ (31,*)CHOISP,COISP
      READ (43,*)CI2G,CHSP,FLRAT,DURTM
      READ (31,*)CIO3SP,CI3SP
      READ (30,*)CDIAM,HEIGHT
C
9     FORMAT('  CONCENTRATION OF THE DROPS',/)
10    FORMAT('AT A TEMPERTURE OF THE GAS ',F6.2,' DEGRESS KELVIN'/
     1 'THE VISCOSITY OF THE LIQUID (CP)=',E15.7/
     2 'THE VISCOSITY OF THE GAS (CP) =',E15.7/
     3 'THE PARTITION COEFFICIENT IS =',E15.7/
     4 'THE DENSITY OF THE LIQUID (GMS/CC) =',E15.7/
     5 'THE DENSITY OF THE GAS (GMS/CC) =',E15.7)
11    FORMAT('THE DIFFUSION COEFFICIENT FOR THE GAS (SQ CM/SEC)=',E15.7
     1 /'THE DIFFUSION COEFFICIENT FOR THE LIQUID (SQ CM/SEC)=',E15.7/
     2 'THE GAS-SIDE MASS TRANSFER COEFFICIENT (CM/SEC)='E15.7/
     3 'THE LIQUID-SIDE MASS TRANSFER COEFFICIENT (CM/SEC)=',E15.7/
     4'THE OVERALL LIQUID-SIDE MASS TRANSFER COEFFICIENT (CM/SEC)=',E15.
     57,/, 'THE VOLUME FOR ONE DROP (LITERS)=',E15.7/
     6 'THE SURFACE AREA FOR ONE DROP (SQ CM)=',E15.7/
     7 'THE EXPOSURE TIME FOR THE DROP IS (SEC)=',E15.7/
     8 'THE REYNOLDS NUMBER FOR THE DROP =',E15.7/
     9 'THE TERMINAL VELOCITY OF THE DROP (CM/SEC) =',E15.7)
```

```
12    FORMAT(I5)
13    FORMAT('                        I2 = ',E15.7/
     2'                      I- = ',E15.7/
     3'                     HOI = ',E15.7/
     4'                    IO3- = ',E15.7/
     5'                      H+ = ',E15.7/
     6'                     IO- = ',E15.7/
     7'                     I3- = ',E15.7/)
14    FORMAT('THE FINAL CONCENTRATION OF THE LIQUID IS (MOLES/LITER) :')
15    FORMAT('THE NUMBER OF MOLES OF IODINE (I2) REMOVED IS =',E15.7,/
     1      'THE NUMBER OF GRAMS OF IODINE REMOVES IS =',E15.7,/)
16    FORMAT('THE FINAL CONCENTRATION OF IODINE (I2) IN THE GAS IS ',
     1E15.7,' (MOLES/LITER)',/)
17    FORMAT('      TIME          MOLES RMD        CON GAS       SUM MLS RM
     1D',/)
18    FORMAT('    CONCENTRATION OF THE SPRAYED SOLUTION IN THE SUMP ',/)
19    FORMAT('    N      TIME          I2             I-             HOI
     1    IO3-            H+            IO-            I3-',/)
21    FORMAT('STEP SIZE BELOW STEP MIN',D15.7)
22    FORMAT(I5,8D13.7)
23    FORMAT(4D15.7)
32    FORMAT('THE NUMBER OF DROPS IN THE CONTAINMENT IS',E15.7/
     1 'THE DROP FLUX (NUMBER OF DROPS/SQ CM MIN) =',E15.7/
     2 'THE CONTAINMENT VOLUME (LITERS) =',E15.7/
     3 'THE NUMBER OF OUTER LOOPS =',I6/)
33    FORMAT(/' THE NUMBER OF GRAMS OF IODINE REMOVED IN THE EXPERIMENT
     1IS ',E15.7,/,'RESULTING IN AN ERROR OF ',E15.7,' PERCENT.'/)
34    FORMAT(//'THE INITIAL CONCENTRATION IN THE GAS OF',E15.7,
     1' (MOLES/LITER)',/,
     2'THE DURATION OF THE SPRAY (MIN) ',E15.7,/,
     3'THE VOLUME OF LIQUID SPRAYED (LITERS) ',E15.7,/,
     4'AND A SPRAY FLOW RATE OF ',E15.7,' (LITERS/MIN)',/,
     5'THE INITIAL CONCENTRATION OF THE LIQUID (MOLES/LITER) :')
C
      WRITE(50,9)
      WRITE(50,19)
      WRITE(52,18)
      WRITE(52,19)
      WRITE(51,17)
C
      SFA=3.1416D00*SAD**2
      VOLD=(3.1416D00*DIAM**3.D00)/(6.D00*1.0D3)
      CI2GI=CI2G
C
      TEMPG4=TEMPG**4
      TEMPG3=TEMPG**3
      TEMPG2=TEMPG**2
C
      TEMPL4=TEMPL**4
      TEMPL3=TEMPL**3
      TEMPL2=TEMPL**2
C
      VSL1=1.8662866D-8*TEMPL4-2.6333695D-5*TEMPL3+1.3970607D-2*TEMPL2
      VSL2=-3.3074806D00*TEMPL+2.9558666D2
      VISLIQ=VSL1+VSL2
C
      PC1=9.981476D-7*TEMPL4-1.5730121D-3*TEMPL3+9.2785676D-1*TEMPL2
      PC2=-2.4288388D2*TEMPL+2.3824847D4
      PC=PC1+PC2
C
      DNL1=6.0251147D-9*TEMPL3-9.1329604D-6*TEMPL2
      DNL2=3.573572D-3*TEMPL+5.8358882D-1
      DENLIQ=DNL1+DNL2
C
      VSA1=-2.8713293D-15*TEMPG4+1.6909463D-11*TEMPG3-4.015468D-8*TEMPG2
      VSA2=6.5679429D-5*TEMPG+1.9523691D-3
      VISGAS=VSA1+VSA2
```

```
      TMP=5.178D-3*TEMPG
C
      OMEGA1=TMP**3*(-6.19047619D-2)+4.657142857D-1*TMP**2
      OMEGA2=TMP*(-1.304238095D00)+2.315428571D00
      OMEGA=OMEGA1+OMEGA2
C
      MLWT=1/2.9D1+1/2.53809D2
C
      DIFGAS=1.858D-3*TEMPG**1.5*MLWT**0.5/(PRESS*4.4355D00**2*OMEGA)
C
      DIFLIQ=3.91D-8*TEMPL/VISLIQ
C
      DNG1=8.2892055D-16*TEMPG4-4.2656962D-12*TEMPG3+8.0228283D-9*TEMPG2
      DNG2=-6.8325529D-6*TEMPG+2.6129391D-3
      DENGAS=DNG1+DNG2
C
      GSM1=0.83D00*((DENLIQ-DENGAS)/DENGAS)**0.25*9.81D2**0.25
      GSM2=(VISGAS/(1.0D2*DENGAS))**-0.17*DIFGAS**0.67*DIAM**-0.25
      KGI2=GSM1*GSM2
C
      ND1=4.D00*DENGAS*(DENLIQ-DENGAS)*9.81D2*DIAM**3
      ND2=3.0D00*(VISGAS/1.0D2)**2
      ND=ND1/ND2
      WW=DLOG10(ND)
C
      NRE1=(-1.81391D00+1.34671D00*WW-0.12427D00*WW**2+6.344D-3*WW**3)
      NRE=1.0D1**NRE1
C
      TRAVEL=NRE*(VISGAS/1.0D2)/(DIAM*DENGAS)
C
      EXPTM=HEIGHT*1.0D2/TRAVEL
C
      KLI2O=(4.0D00*DIFLIQ*TRAVEL/(3.1415D00*DIAM))**0.5
C
      KLOV=KGI2*KLI2O/(PC*KLI2O+KGI2)
C
      CCSA=(CDIAM/2.0D00)**2.0*3.14149265D00
C
      DPMIN=FLRAT/VOLD
C
      FLIDP=DPMIN/(CCSA*1.0D4)
C
      ADARA=6.0D1/(EXPTM*FLIDP)
C
      ILOOP=DURTM*6.0D1/EXPTM+1.0D00
C
      VOLCON=ADARA*HEIGHT/1.0D1
C
      VOLSP=FLRAT*DURTM
C
      NUMDPS=DPMIN*EXPTM/6.0D1
C
      CVOL=CCSA*HEIGHT*1.0D3
C
      WRITE(23,12)ILOOP
      WRITE (22,10) TEMPG,VISLIQ,VISGAS,PC,DENLIQ,DENGAS
      WRITE (22,11) DIFGAS,DIFLIQ,KGI2,KLI2O,KLOV,VOLD,SFA,EXPTM,NRE,
     1              TRAVEL
      WRITE (22,32)NUMDPS,FLIDP,CVOL,ILOOP
      WRITE (22,34)CI2G,DURTM,VOLSP,FLRAT
C
C     DETERMINE THE EQUILIBRIUM CONSTANTS FOR K4, K5 AND K6
C
      RK6=-4.098D00-3245.2D00/TEMPL+2.2363D5/(TEMPL**2)-3.984D7/(TEMPL**
     13)+(13.957D00-1262.3D00/TEMPL+8.5641D5/(TEMPL**2))*DLOG(DENLIQ)
      RK6=10**(RK6)
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```
      RK5=10**(2800.48D00+0.7335D00*TEMPL-80670.0D00/TEMPL
     1-1115.1D00*DLOG10(TEMPL))
C
      RK4=DEXP(3727.86D00/TEMPL-11.6326D00+0.0192212D00*TEMPL)
C
      TOUTPL=EXPTM/2.0D1
      SPA=SPA*NUMDPS
      VOLD=NUMDPS*VOLD
      TOLD=A
      Q=1.0D-1
C
      WRITE (22,13)CI2SP,CISP,CHOISP,CIO3SP,CHSP,COISP,CI3SP
      WRITE(50,22) I,TIME,WOLD(1),WOLD(2),WOLD(3),WOLD(4),WOLD(5),WOLD(6)
     1              ,WOLD(7)
C
      DO 1100 II=1,ILOOP
      IMK=IMK+1.0D00
      H=1.0D-2
      TOLD=A
      B=EXPTM
      CI2G=((CI2G*CVOL)-SUMMOL)/CVOL
      CI2L=CI2SP
C
C     INITIALIZE THE SPRAY DROPS
C
      WOLD(2)=CISP
      WOLD(5)=CHSP
      WOLD(4)=CIO3SP
      WOLD(7)=CI3SP
      WOLD(3)=CHOISP
      WOLD(6)=COISP
      WOLD(8)=RK6/WOLD(5)
C
      SUMMOL=0.0D00
C
C     BEGIN THE RUNGE-KUTTA-FELBBURG INTEGRATION ROUTINE
C
1     T=TOLD
C
C     DETERMINE THE MASS TRANSFER TO THE SPRAY DROPLETS
C
      WOLD(1)=CI2L
      NMOL=WOLD(1)*VOLD
      MOLTR=KLOV*H*SPA*(CI2G*PC-WOLD(1))/1.0D3
      WOLD(1)=(NMOL+MOLTR)/VOLD
C
C     CALCULATE K'S
C
      DO 30 J=1,IN
       W(J)=WOLD(J)
30    CONTINUE
C
      CALL FUNCTN(W,WOLD,F,IN)
C
      DO 40 J=1,IN
       K1(J)=H*F(J)
40    CONTINUE
C
      DO 50 J=1,IN
       W(J)=WOLD(J)+K1(J)/4.0D00
50    CONTINUE
C
      CALL FUNCTN(W,WOLD,F,IN)
C
      DO 60 J=1,IN
       K2(J)=H*F(J)
```

```
60    CONTINUE
C
      DO 80 J=1,IN
       W(J)=WOLD(J)+3.0D00*K1(J)/3.2D1+9.0D00*K2(J)/3.2D1
80    CONTINUE
C
      CALL FUNCTN(W,WOLD,F,IN)
C
      DO 90 J=1,IN
       K3(J)=H*F(J)
90    CONTINUE
C
      DO 110 J=1,IN
       W(J)=WOLD(J)+1.932D3*K1(J)/2.197D3-7.2D3*K2(J)/2.197D3
     1      +7.296D3*K3(J)/2.197D3
110   CONTINUE
C
      CALL FUNCTN(W,WOLD,F,IN)
C
      DO 120 J=1,IN
       K4(J)=H*F(J)
120   CONTINUE
C
      DO 130 J=1,IN
       W(J)=WOLD(J)+4.39D2*K1(J)/2.16D2-8.0D00*K2(J)+3.68D3*K3(J)/5.13D2
     1      -8.45D2*K4(J)/4.104D3
130   CONTINUE
C
      CALL FUNCTN(W,WOLD,F,IN)
C
      DO 140 J=1,IN
       K5(J)=H*F(J)
140   CONTINUE
C
      DO 150 J=1,IN
       W(J)=WOLD(J)-8.D00*K1(J)/2.7D1+2.D00*K2(J)-3.544D3*K3(J)/2.565D3
     1      +1.859D3*K4(J)/4.104D3-1.1D1*K5(J)/4.0D1
150   CONTINUE
C
      CALL FUNCTN(W,WOLD,F,IN)
C
      DO 160 J=1,IN
       K6(J)=H*F(J)
160   CONTINUE
C
C
C     DETERMINE THE CONCENTRATION OF ALL IODINE HYDROLYSIS SPECIES
C     AND CHECK ERROR
C
      DO 100 J=1,IN
       WB(J)=WOLD(J)+1.6D1*K1(J)/1.35D2+6.656D3*K3(J)/1.2825D4+
     1       2.8561D4*K4(J)/5.643D4-9.0D00*K5(J)/5.0D1+2.0D00*K6(J)/5.5D1
       R(J)=ABS(K1(J)/3.6D2-1.28D2*K3(J)/4.275D3-2.197D3*K4(J)/7.524D4
     1          +K5(J)/5.0D1+2.0D00*K6(J)/5.5D1)/H
       TOL(J)=ABS(WB(J)*TOLER)
       DELTA(J)=0.84*(TOL(J)/R(J))**0.25
100   CONTINUE
C
      DO 500 J=1,IN
       IF(R(J) .GT. TOL(J))GOTO 900
500   CONTINUE
C
      DO 510 J=1,IN
       WOLD(J)=WB(J)
510   CONTINUE
C
```

```
C     DETERMINE THE EQUILIBRIUM CONCENTRATION FOR EQUATIONS 23, 24 AND
C     25
C
      BB=-1.0D00-(WOLD(2)+WOLD(1))*RK4
      C=WOLD(2)*WOLD(1)*RK4-WOLD(7)
      D=-BB/(2.0D00*RK4)
      E=((BB**2.0D00-4.0D00*RK4*C)**0.5D00)/(2.0D00*RK4)
      V=D-E
C
      IF(V .LT. 1.0D-18 .AND. V .NE. 0.0D00) CALL ITTER(WOLD,RK4,C,V)
C
      WOLD(7)=WOLD(7)+V
      WOLD(1)=WOLD(1)-V
      WOLD(2)=WOLD(2)-V
C
      IF(IN .EQ. 4)GOTO 600
C
      RR=WOLD(6)+WOLD(5)+RK5
      S=-RK5*WOLD(3)+WOLD(6)*WOLD(5)
      H=(-RR+(RR*RR-4.0D00*S)**0.5)/2.0D00
      WOLD(5)=WOLD(5)+H
      GOTO 605
C
600   H=(RK5*WOLD(3)-WOLD(6)*WOLD(5))/(WOLD(5)+RK5)
C
605   WOLD(6)=WOLD(6)+H
      WOLD(3)=WOLD(3)-H
C
      IF(IN .EQ. 4)GOTO 615
C
      U=WOLD(8)*WOLD(5)-RK6
      VV=WOLD(8)+WOLD(5)
      X=(-VV+(VV*VV-4.0D00*U)**0.5)/2.0D00
      WOLD(5)=WOLD(5)+X
      WOLD(8)=WOLD(8)+X
C
615   TOLD=TOLD+H
      SUMMOL=SUMMOL+MOLTR
      FHT=TRAVEL*TIME
      CI2L=WB(1)
      FHT=TOLD*TRAVEL
      DEL=DELTA(1)
      IF(IN .EQ. 1)GOTO 905
C
      DO 520 J=2,IN
       IF(DEL .LT. DELTA(J))GOTO 520
       DEL=DELTA(J)
520   CONTINUE
C
      GOTO 905
C
C     DETERMINE NEW STEP SIZE
C
900   DEL=DELTA(J)
C
905   IF(DEL .GT. Q)GOTO 910
      HNEW=Q*H
      GOTO 1000
C
910   IF(DEL .LT. 4.0)GOTO 920
      HNEW=4.0D00*H
      GOTO 1000
C
920   HNEW=DEL*H
C
C     CHECK NEW STEP SIZE WITH MAX AND MIN STEP SIZE
```

```
C
1000  IF (HNEW .LT. HMAX) GOTO 930
      HNEW=HMAX
C
930   IF (HNEW .LT. HMIN) GOTO 1111
      LEFT=B-TOLD-HNEW
C
      IF(LEFT .GT. 0.0) GOTO 5000
      HNEW=B-TOLD
C
5000  H=HNEW
C
      IF(TOLD .GE. B) GOTO 999
      GOTO 1
C
C
999   SUM=SUM+SUMMOL
      TIME=TIME+TOLD/6.0D1
      FHT=TIME*TRMVEL
      H=1.0D-2
      TOLD=A
C
      WRITE(50,22) II,TIME,WOLD(1),WOLD(2),WOLD(3),WOLD(4),WOLD(5),
     1             WOLD(6),WOLD(7)
      WRITE(51,23) TIME,SUMMOL,CI2G,SUM
C
C     DETERMINE THE CONCENTRATION IN THE SUMP
C
C     BEGIN RUNGE-KUTTA-FELBERG INTEGRATION ROUTINE
C
C     CALCULATE K'S
C
2     DO 31 J=1,IN
       CC(J)=CONPOL(J)
31    CONTINUE
C
      CALL FUNCTN(CC,CONPOL,F,IN)
C
      DO 41 J=1,IN
       K1(J)=H*F(J)
41    CONTINUE
C
      DO 51 J=1,IN
       CC(J)=CONPOL(J)+K1(J)/4.0D00
51    CONTINUE
C
      CALL FUNCTN(CC,CONPOL,F,IN)
C
      DO 61 J=1,IN
       K2(J)=H*F(J)
61    CONTINUE
C
      DO 81 J=1,IN
       CC(J)=CONPOL(J)+3.0D00*K1(J)/3.2D1+9.0D00*K2(J)/3.2D1
81    CONTINUE
C
      CALL FUNCTN(CC,CONPOL,F,IN)
C
      DO 91 J=1,IN
       K3(J)=H*F(J)
91    CONTINUE
C
      DO 111 J=1,IN
       CC(J)=CONPOL(J)+1.932D3*K1(J)/2.197D3-7.2D3*K2(J)/2.197D3
     1       +7.296D3*K3(J)/2.197D3
111   CONTINUE
```

```
C
      CALL FUNCTN(CC,CONPOL,F,IN)
C
      DO 121 J=1,IN
       K4(J)=H*F(J)
121   CONTINUE
C
      DO 131 J=1,IN
       CC(J)=CONPOL(J)+4.39D2*K1(J)/2.16D2-8.0D00*K2(J)+
     1      3.68D3*K3(J)/5.13D2-8.45D2*K4(J)/4.104D3
131   CONTINUE
C
      CALL FUNCTN(CC,CONPOL,F,IN)
C
      DO 141 J=1,IN
       K5(J)=H*F(J)
141   CONTINUE
C
      DO 151 J=1,IN
       CC(J)=CONPOL(J)-8.0D00*K1(J)/2.7D1+2.0D00*K2(J)-
     1     3.544D3*K3(J)/2.565D3+1.859D3*K4(J)/4.104D3-1.1D1*K5(J)/4.0D1
151   CONTINUE
C
      CALL FUNCTN(CC,CONPOL,F,IN)
C
      DO 161 J=1,IN
       K6(J)=H*F(J)
161   CONTINUE
C
C     DETERMINE THE CONCENTRATION OF ALL OF THE IODINE HYDROLYSIS
C     SPECIES AND CHECK ERROR
C
      DO 101 J=1,IN
       CCB(J)=CONPOL(J)+1.6D1*K1(J)/1.35D2+6.656D3*K3(J)/1.2825D4+
     1       2.8561D4*K4(J)/5.643D4-9.0D00*K5(J)/5.0D1+2.0D00*K6(J)/5.5D1
       R(J)=ABS(K1(J)/3.6D2-1.28D2*K3(J)/4.275D3-2.197D3*K4(J)/7.524D4
     1           +K5(J)/5.0D1+2.0D00*K6(J)/5.5D1)/H
       TOL(J)=ABS(CCB(J)*TOLER)
       DELTA(J)=0.84*(TOL(J)/R(J))**0.25
101   CONTINUE
C
      DO 501 J=1,IN
       IF(R(J) .GT. TOL(J))GOTO 901
501   CONTINUE
C
      DO 511 J=1,IN
       CONPOL(J)=CCB(J)
511   CONTINUE
C
C     DETERMINE THE EQUILIBRIUM CONCENTRATION FOR EQUATIONS 23, 24 AND
C     25
C
      BB=-1.0D00-(CONPOL(2)+CONPOL(1))*RK4
      C=CONPOL(2)*CONPOL(1)*RK4-CONPOL(7)
      D=-BB/(2.0D00*RK4)
      E=((BB**2.0D00-4.0D00*RK4*C)**0.5D00)/(2.0D00*RK4)
      V=D-E
C
666   IF(V .LT. 1.0D-18 .AND. V .NE. 0.0D00)CALL ITTER(CONPOL,RK4,C,V)
C
      CONPOL(7)=CONPOL(7)+V
      CONPOL(1)=CONPOL(1)-V
      CONPOL(2)=CONPOL(2)-V
C
      IF(IN .EQ. 4)GOTO 601
C
```

```
      RR=CONPOL(6)+CONPOL(5)+RK5
      S=-RK5*CONPOL(3)+CONPOL(6)*CONPOL(5)
      H=(-RR+(RR*RR-4.0D00*S)**0.5)/2.0D00
      CONPOL(5)=CONPOL(5)+H
      GOTO 606
C
601   H=(RK5*CONPOL(3)-CONPOL(6)*CONPOL(5))/(CONPOL(5)+RK5)
C
606   CONPOL(6)=CONPOL(6)+H
      CONPOL(3)=CONPOL(3)-H
C
      IF(IN .EQ. 1)GOTO 616
C
      U=CONPOL(8)*CONPOL(5)-RK6
      VV=CONPOL(8)+CONPOL(5)
      X=(-VV+(VV*VV-4.0D00*U)**0.5)/2.0D00
      CONPOL(5)=CONPOL(5)+X
      CONPOL(8)=CONPOL(8)+X
C
616   TOLD=TOLD+H
C
      DEL=DELTA(1)
C
      IF(IN .EQ. 1)GOTO 906
C
      DO 521 J=2,IN
       IF(DEL .LT. DELTA(J))GOTO 521
       DEL=DELTA(J)
521   CONTINUE
C
      GOTO 906
C
C     DETERMINE NEW STEP SIZE
C
901   DEL=DELTA(J)
C
906   IF(DEL .GT. Q)GOTO 911
      HNEW=Q*H
      GOTO 1001
C
911   IF(DEL .LT. 4.0)GOTO 921
      HNEW=4.0D00*H
      GOTO 1001
C
921   HNEW=DEL*H
C
C     CHECK NEW STEP SIZE WITH MAX AND MIN STEP SIZE
C
1001  IF (HNEW .LT. HMAX)GOTO 931
      HNEW=HMAX
C
931   IF (HNEW .LT. HMIN)GOTO 1112
      LEFT=B-TOLD-HNEW
C
      IF(LEFT .GT. 0.0)GOTO 5001
      HNEW=B-TOLD
C
5001  H=HNEW
C
      IF(TOLD .GE. B)GOTO 998
C
      GOTO 2
C
998   DO 800 IQ=1,7
C
800   CONPOL(IQ)=(WOLD(IQ)*VOLD+CONPOL(IQ)*POLVOL)/(POLVOL+VOLD)
```

```
      POLVCL=POLVCL+VOLD
C
      WRITE(52,22) II,TIME,CONPOL(1),CONPOL(2),CONPOL(3),CONPOL(4),
     1             CONPOL(5),CONPOL(6),CONPOL(7)
C
1100  CONTINUE
C
      SUMGRM=2.53809D2*SUM
C
      WRITE(22,16) CI2G
      WRITE(22,15) SUM,SUMGRM
      WRITE(22,14)
      WRITE(22,13) CONPOL(1),CONPOL(2),CONPOL(3),CONPOL(4),CONPOL(5),
     1             CONPOL(6),CONPOL(7)
C
      GOTO 3000
C
1111  WRITE(40,21) HNEW
1112  WRITE(40,21) HNEW
3000  STOP
C
      END
```

```
C***********************************************************************
C
C     SUBROUTINE FUNCTN
C
C     THIS SUBROUTINE CONTAINS THE DIFFERENTIAL EQUATIONS (KINETIC RATE
C     EQUATIONS) TO BE INTEGRATED.  THIS SUBROUTINE IS CALLED FROM THE
C     RUNGE-KUTTA-FELHBURG INTEGRATION ROUTINE IN THE KINETIC, DROP,
C     SPRAY AND WALL-SPRAY MODELS.
C
C***********************************************************************
C
      SUBROUTINE FUNCTN (W,WOLD,F,IN)
C
      IMPLICIT DOUBLE PRECISION(A-H,K-Z)
      IMPLICIT INTEGER (I-J)
C
      DIMENSION W(8),WOLD(8),F(7)
C
      IF(IN .EQ. 5)GOTO 5
C
      W(5)=WOLD(5)
5     W(6)=WOLD(6)
C
      RK1=3.0D00
      RKR1=4.4D12
      RK20=2.5D02
      RK21=1.2D02
      RKR2=3.0D08
      RKP3=9.35D-8
C
      R1=RK1*W(1)
      RR1=RKR1*W(2)*W(3)*W(5)
      R20=RK20*W(3)**2.0D00
      R21=RK21*W(3)*W(6)
      RR2=RKR2*W(4)*W(2)**2.0D00*W(5)**2.0D00
      RP3=RKP3*W(5)*W(2)
C
      F(1)=-R1+RR1+5.0D-1*RP3
      F(2)=R1-RR1+2.0D00*(R20+R21)/3.0D00-2.0D00*RR2-RP3
      F(3)=R1-RR1-R20-R21+3.0D00*RR2
      F(4)=(R20+R21)/3.0D00-RR2
C
      IF (IN .EQ. 5)GOTO 10
C
      F(5)=0.0D00
      GOTO 11
C
10    F(5)=R1-RR1+R20+R21-3.0D00*RR2-4.0D00*RP3
C
11    F(6)=0.0D00
      F(7)=0.0D00
C
      RETURN
C
      END
```

```
C***********************************************************************
C
C     SUBROUTINE ITTER
C
C     THIS SUBROUTINE FINDS THE ROOT TO THE QUADRATIC EQUILIBRIUM
C     EQUATION FOR THE FORMATION REACTION OF TRI-IODIDE, I3- (EQUATION
C     23).  A SECANT METHOD IS THE ROUTINE USED TO FIND THE ROOT.  THIS
C     METHOD IS CALLED WHENEVER THE QUADRATIC FORMULA RESULTS IN LESS
C     THAN APPROXIMATELY THREE SIGNIFICANT FIGURES.  THIS SUBROUTINE
C     IS CALLED BY THE PROGRAMS KINETIC, DROP, SPRAY AND WALL-SPRAY.
C
C***********************************************************************
C
      SUBROUTINE ITTER(WOLD,RK4,C,V)
C
      IMPLICIT DOUBLE PRECISION (A-H,L-Z)
      IMPLICIT INTEGER (I-K)
C
      DIMENSION WOLD(7),W(7)
C
      P0=1.0D-16
      P1=1.0D-18
C
      Q0=C-RK4*P0*P0-P0*RK4*(WOLD(1)+WOLD(2))-P0
5     Q1=C-RK4*P1*P1-P1*RK4*(WOLD(1)+WOLD(2))-P1
C
      NEW=P1-Q1*(P1-P0)/(Q1-Q0)
C
      CHECK=ABS(NEW-P1)/P1
C
11    IF (CHECK .LT. 1.0D-4) GOTO 10
C
      P0=P1
      Q0=Q1
      P1=NEW
      GOTO 5
C
10    V=NEW
C
      RETURN
C
      END
```

Spray Model sample input

A = 0.0

B = DURTM = 10

HMIN = 1.0×10^{-10}

HMAX = 1.0×10^{2}

IN = 4

TOLER = 1.0×10^{-2}

TEMPL = 298

TEMPG = 298

DIAM = 0.1

SAD = 0.1

CI2G = 1.0×10^{-5}

CI2SP = 0.0

CISP = 0.0

CHOISP = 0.0

COISP = 0.0

CHSP = 1.0×10^{-9}

CIO3SP = 0.0

CI3SP = 0.0

PRESS = 1.0

CDIAM = 3.3

HEIGHT = 15.4

FLRAT = 37

```
AT A TEMPERTURE OF THE GAS 298.00 DEGREES KELVIN
THE VISCOSITY OF THE LIQUID (CP)=  0.8972334E+00
THE VISCOSITY OF THE GAS (CP) =  0.1838378E-01
THE PARTITION COEFFICIENT IS =  0.8683416E+02
THE DENSITY OF THE LIQUID (GMS/CC) =  0.9969160E+00
THE DENSITY OF THE GAS (GMS/CC) =  0.1182949E-02
THE DIFFUSION COEFFICIENT FOR THE GAS (SQ CM/SEC)=  0.8040764E-01
THE DIFFUSION COEFFICIENT FOR THE LIQUID (SQ CM/SEC)=  0.1298637E-04
THE GAS-SIDE MASS TRANSFER COEFFICIENT (CM/SEC)=  0.1127948E+02
THE LIQUID-SIDE MASS TRANSFER COEFFICIENT (CM/SEC)=  0.2553658E+00
THE OVERALL LIQUID-SIDE MASS TRANSFER COEFFICIENT (CM/SEC)=  0.8610024E-01
THE VOLUME FOR ONE DROP (LITERS)=  0.5236000E-06
THE SURFACE AREA FOR ONE DROP (SQ CM)=  0.3141600E-01
THE EXPOSURE TIME FOR THE DROP IS (SEC)=  0.3904862E+01
THE REYNOLDS NUMBER FOR THE DROP =  0.2537734E+03
THE TERMINAL VELOCITY OF THE DROP (CM/SEC) =  0.3943801E+03
THE NUMBER OF DROPS IN THE CONTAINMENT IS  0.4723222E+07
THE DROP FLUX (NUMBER OF DROPS/SQ CM MIN) =  0.8247353E+03
THE CONTAINMENT VOLUME (LITERS) =  0.1355156E+06
THE NUMBER OF OUTER LOOPS =   154
THE INITIAL CONCENTRATION IN THE GAS OF  0.1000000E-04 (MOLES/LITER)
THE DURATION OF THE SPRAY (MIN)   0.1000000E+02
THE VOLUME OF LIQUID SPRAYED (LITERS)   0.3800000E+03
AND A SPRAY FLOW RATE OF   0.3800000E+02 (LITERS/MIN)
THE INITIAL CONCENTRATION OF THE LIQUID (MOLES/LITER) :
                    I2 =   0.0000000E+00
                    I- =   0.0000000E+00
                   HOI =   0.0000000E+00
                  IO3- =   0.0000000E+00
                    H+ =   0.1000000E-08
                   IO- =   0.0000000E+00
                   I3- =   0.0000000E+00
THE FINAL CONCENTRATION OF IODINE (I2) IN THE GAS IS   0.5597029E-05 (MOLES/LITER)
THE NUMBER OF MOLES OF IODINE (I2) REMOVED IS =  0.5996871E+00
THE NUMBER OF GRAMS OF IODINE REMOVES IS =  0.1522060E+03
THE FINAL CONCENTRATION OF THE LIQUID IS (MOLES/LITER) :
                    I2 =   0.2288953E-03
                    I- =   0.1939883E-02
                   HOI =   0.8201864E-04
                  IO3- =   0.4364906E-03
                    H+ =   0.1000000E-08
                   IO- =   0.1877840E-05
                   I3- =   0.3264659E-03
```

FOR50

DAT

File: DSKB:FOR50.DAT[6452,232] Created: 07-Oct-84 16:55:00 <055> Printed: 07-Oct-84 16:56:53
QUEUE Switches: /FILE:FORT /COPIES:1 /SPACING:1 /LIMIT:276

CONCENTRATION OF THE DROPS

N	TIME	I2	I-	HOI	IO3-	H+	IO-	I3-
0	.0000000D+00	.0000000D+00	.0000000D+00	.0000000D+00	.0000000D+00	.0000000D+00	.0000000D+00	.0000000D+00
1	.6508103D-01	.8540259D-03	.8872849D-03	.6453274D-03	.1573912D-03	.1000000D-08	.1477495D-04	.5597734D-03
2	.1301621D+00	.8511840D-03	.8856122D-03	.6441550D-03	.1567136D-03	.1000000D-08	.1474811D-04	.5568589D-03
3	.1952431D+00	.8483514D-03	.8839358D-03	.6429822D-03	.1560388D-03	.1000000D-08	.1472126D-04	.5539577D-03
4	.2603241D+00	.8455280D-03	.8822679D-03	.6418090D-03	.1553669D-03	.1000000D-08	.1469440D-04	.5510698D-03
5	.3254052D+00	.8427135D-03	.8805968D-03	.6406359D-03	.1546977D-03	.1000000D-08	.1466754D-04	.5481951D-03
6	.3904862D+00	.8399074D-03	.8789266D-03	.6394630D-03	.1540313D-03	.1000000D-08	.1464068D-04	.5453335D-03
7	.4555672D+00	.8371096D-03	.9772579D-03	.6382908D-03	.1533677D-03	.1000000D-08	.1461385D-04	.5424850D-03
8	.5206483D+00	.8343185D-03	.8755914D-03	.6371196D-03	.1527068D-03	.1000000D-08	.1458703D-04	.5396491D-03
9	.5857293D+00	.8315347D-03	.8739271D-03	.6359500D-03	.1520486D-03	.1000000D-08	.1456025D-04	.5368262D-03
10	.6508103D+00	.8287577D-03	.8722656D-03	.6347825D-03	.1513932D-03	.1000000D-08	.1453352D-04	.5340162D-03
11	.7158914D+00	.8215807D-03	.8723757D-03	.6336257D-03	.1507403D-03	.1000000D-08	.1450704D-04	.5294584D-03
12	.7809724D+00	.8188101D-03	.8707384D-03	.6324915D-03	.1500897D-03	.1000000D-08	.1448107D-04	.5266826D-03
13	.8460534D+00	.8160477D-03	.8691023D-03	.6313576D-03	.1494418D-03	.1000000D-08	.1445511D-04	.5239195D-03
14	.9111344D+00	.8132939D-03	.8674671D-03	.6302240D-03	.1487966D-03	.1000000D-08	.1442915D-04	.5211691D-03
15	.9762155D+00	.8105489D-03	.8658325D-03	.6290902D-03	.1481541D-03	.1000000D-08	.1440320D-04	.5184313D-03
16	.1041297D+01	.8078126D-03	.8641984D-03	.6279563D-03	.1475142D-03	.1000000D-08	.1437723D-04	.5157060D-03
17	.1106378D+01	.8050852D-03	.8625648D-03	.6268220D-03	.1468770D-03	.1000000D-08	.1435127D-04	.5129933D-03
18	.1171459D+01	.8023668D-03	.8609316D-03	.6256874D-03	.1462424D-03	.1000000D-08	.1432529D-04	.5102931D-03
19	.1236540D+01	.7996572D-03	.8592988D-03	.6245526D-03	.1456104D-03	.1000000D-08	.1429931D-04	.5076053D-03
20	.1301621D+01	.7969563D-03	.8576664D-03	.6234174D-03	.1449811D-03	.1000000D-08	.1427332D-04	.5049298D-03
21	.1366702D+01	.7942641D-03	.8560347D-03	.6222822D-03	.1443544D-03	.1000000D-08	.1424732D-04	.5022667D-03
22	.1431783D+01	.7915805D-03	.8544036D-03	.6211469D-03	.1437302D-03	.1000000D-08	.1422133D-04	.4996159D-03
23	.1496864D+01	.7889051D-03	.8527734D-03	.6200118D-03	.1431087D-03	.1000000D-08	.1419534D-04	.4969773D-03
24	.1561945D+01	.7862378D-03	.8511444D-03	.6188772D-03	.1424897D-03	.1000000D-08	.14[illegible]6937D-04	.4943508D-03
25	.1627026D+01	.7835783D-03	.8495167D-03	.6177432D-03	.1418733D-03	.1000000D-08	.1414340D-04	.4917364D-03
26	.1692107D+01	.7809263D-03	.3478907D-03	.6166102D-03	.1412594D-03	.1000000D-08	.1411746D-04	.4891341D-03
27	.1757188D+01	.7782814D-03	.8462666D-03	.6154785D-03	.1406481D-03	.1000000D-08	.1409155D-04	.4865438D-03
28	.1822269D+01	.7756432D-03	.8446450D-03	.6143485D-03	.1400393D-03	.1000000D-08	.1406568D-04	.4839654D-03
29	.1887350D+01	.7730114D-03	.8430263D-03	.6132207D-03	.1394329D-03	.1000000D-08	.1403986D-04	.4813989D-03
30	.1952431D+01	.7703853D-03	.8414108D-03	.6120955D-03	.1388291D-03	.1000000D-08	.1401410D-04	.4788441D-03
31	.2017512D+01	.7637213D-03	.8414090D-03	.6109842D-03	.1382274D-03	.1000000D-08	.1398865D-04	.4747010D-03
32	.2082593D+01	.7611080D-03	.8398097D-03	.6098836D-03	.1376280D-03	.1000000D-08	.1396345D-04	.4721775D-03
33	.2147674D+01	.7585020D-03	.8382119D-03	.6087836D-03	.1370311D-03	.1000000D-08	.1393827D-04	.4696655D-03
34	.2212755D+01	.7559039D-03	.8366152D-03	.6076841D-03	.1364366D-03	.1000000D-08	.1391310D-04	.4671652D-03

35	.2277836D+01	.7533137D-03	.8350195D-03	.6065848D-03	.1358446D-03	.1000000D-08	.1388793D-04	.4646764D-03
36	.2342917D+01	.7507316D-03	.8334247D-03	.6054858D-03	.1352551D-03	.1000000D-08	.1386277D-04	.4621992D-03
37	.2407998D+01	.7481576D-03	.8318306D-03	.6043868D-03	.1346679D-03	.1000000D-08	.1383760D-04	.4597334D-03
38	.2473079D+01	.7455917D-03	.8302373D-03	.6032880D-03	.1340832D-03	.1000000D-08	.1381245D-04	.4572791D-03
39	.2538160D+01	.7430339D-03	.8286447D-03	.6021892D-03	.1335009D-03	.1000000D-08	.1378729D-04	.4548363D-03
40	.2603241D+01	.7404841D-03	.8270530D-03	.6010906D-03	.1329210D-03	.1000000D-08	.1376214D-04	.4524047D-03
41	.2668322D+01	.7379421D-03	.8254622D-03	.5999923D-03	.1323435D-03	.1000000D-08	.1373699D-04	.4499845D-03
42	.2733403D+01	.7354079D-03	.8238724D-03	.5988944D-03	.1317683D-03	.1000000D-08	.1371185D-04	.4475756D-03
43	.2798484D+01	.7328813D-03	.8222838D-03	.5977970D-03	.1311956D-03	.1000000D-08	.1368673D-04	.4451778D-03
44	.2863565D+01	.7303621D-03	.8206966D-03	.5967004D-03	.1306252D-03	.1000000D-08	.1366162D-04	.4427912D-03
45	.2928646D+01	.7278500D-03	.8191111D-03	.5956047D-03	.1300571D-03	.1000000D-08	.1363654D-04	.4404157D-03
46	.2993727D+01	.7253498D-03	.8175273D-03	.5945102D-03	.1294914D-03	.1000000D-08	.1361148D-04	.4380512D-03
47	.3058808D+01	.7228462D-03	.8159458D-03	.5934173D-03	.1289280D-03	.1000000D-08	.1358645D-04	.4356978D-03
48	.3123890D+01	.7203539D-03	.8143667D-03	.5923261D-03	.1283669D-03	.1000000D-08	.1356147D-04	.4333552D-03
49	.3188971D+01	.7178675D-03	.8127905D-03	.5912372D-03	.1278081D-03	.1000000D-08	.1353654D-04	.4310235D-03
50	.3254052D+01	.7153866D-03	.8112175D-03	.5901509D-03	.1272515D-03	.1000000D-08	.1351167D-04	.4287027D-03
51	.3319133D+01	.7129107D-03	.8096482D-03	.5890676D-03	.1266973D-03	.1000000D-08	.1348687D-04	.4263925D-03
52	.3384214D+01	.7104396D-03	.8080832D-03	.5879878D-03	.1261450D-03	.1000000D-08	.1346214D-04	.4240929D-03
53	.3449295D+01	.7079725D-03	.8065231D-03	.5869118D-03	.1255958D-03	.1000000D-08	.1343750D-04	.4218035D-03
54	.3514376D+01	.7055089D-03	.8049686D-03	.5858399D-03	.1250486D-03	.1000000D-08	.1341295D-04	.4195242D-03
55	.3579457D+01	.6994063D-03	.8048543D-03	.5847982D-03	.1245011D-03	.1000000D-08	.1338912D-04	.4158387D-03
56	.3644538D+01	.6969706D-03	.8032977D-03	.5837338D-03	.1239577D-03	.1000000D-08	.1336475D-04	.4135892D-03
57	.3709619D+01	.6945427D-03	.8017422D-03	.5826699D-03	.1234164D-03	.1000000D-08	.1334039D-04	.4113503D-03
58	.3774700D+01	.6921216D-03	.8001880D-03	.5816064D-03	.1228774D-03	.1000000D-08	.1331604D-04	.4091217D-03
59	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	.1000000D-08	[illegible]	[illegible]
60	.3904362D+01	.6872012D-03	.7970827D-03	.5794807D-03	.1218061D-03	.1000000D-08	.1326737D-04	.4046957D-03
61	.3969943D+01	.6849019D-03	.7955318D-03	.5784186D-03	.1212737D-03	.1000000D-08	.1324306D-04	.4024983D-03
62	.4035024D+01	.6825099D-03	.7939820D-03	.5773570D-03	.1207435D-03	.1000000D-08	.1321875D-04	.4003112D-03
63	.4100105D+01	.6801250D-03	.7924334D-03	.5762961D-03	.1202154D-03	.1000000D-08	.1319446D-04	.3981343D-03
64	.4165186D+01	.6777471D-03	.7908863D-03	.5752360D-03	.1196896D-03	.1000000D-08	.1317019D-04	.3959677D-03
65	.4230267D+01	.6753759D-03	.7893408D-03	.5741769D-03	.1191659D-03	.1000000D-08	.1314594D-04	.3938113D-03
66	.4295348D+01	.6730114D-03	.7877970D-03	.5731188D-03	.1186443D-03	.1000000D-08	.1312172D-04	.3916650D-03
67	.4360429D+01	.6706532D-03	.7862551D-03	.5720622D-03	.1181249D-03	.1000000D-08	.1309752D-04	.3895288D-03
68	.4425510D+01	.6683013D-03	.7847155D-03	.5710071D-03	.1176075D-03	.1000000D-08	.1307337D-04	.3874027D-03
69	.4490591D+01	.6659552D-03	.7831783D-03	.5699538D-03	.1170923D-03	.1000000D-08	.1304925D-04	.3852864D-03
70	.4555672D+01	.6636147D-03	.7816438D-03	.5689027D-03	.1165792D-03	.1000000D-08	.1302519D-04	.3831801D-03
71	.4620753D+01	.6612795D-03	.7801125D-03	.5678541D-03	.1160682D-03	.1000000D-08	.1300118D-04	.3810837D-03
72	.4685834D+01	.6589491D-03	.7785846D-03	.5668082D-03	.1155592D-03	.1000000D-08	.1297723D-04	.3789970D-03
73	.4750915D+01	.6566218D-03	.7770611D-03	.5657656D-03	.1150523D-03	.1000000D-08	.1295336D-04	.3769195D-03
74	.4815996D+01	.6509653D-03	.7768324D-03	.5647289D-03	.1145473D-03	.1000000D-08	.1292963D-04	.3735625D-03
75	.4881077D+01	.6486602D-03	.7753118D-03	.5636964D-03	.1140441D-03	.1000000D-08	.1290599D-04	.3715111D-03
76	.4946158D+01	.6463616D-03	.7737928D-03	.5626650D-03	.1135430D-03	.1000000D-08	.1288237D-04	.3694693D-03
77	.5011239D+01	.6440689D-03	.7722757D-03	.5616346D-03	.1130439D-03	.1000000D-08	.1285878D-04	.3674369D-03
78	.5076320D+01	.6417820D-03	.7707603D-03	.5606050D-03	.1125468D-03	.1000000D-08	.1283521D-04	.3654138D-03
79	.5141402D+01	.6395018D-03	.7692463D-03	.5595763D-03	.1120517D-03	.1000000D-08	.1281165D-04	.3634003D-03
80	.5206483D+01	.6372284D-03	.7677336D-03	.5585483D-03	.1115587D-03	.1000000D-08	.1278812D-04	.3613964D-03
81	.5271564D+01	.6349614D-03	.7662224D-03	.5575210D-03	.1110677D-03	.1000000D-08	.1276460D-04	.3594018D-03
82	.5336645D+01	.6326997D-03	.7647130D-03	.5564945D-03	.1105787D-03	.1000000D-08	.1274110D-04	.3574162D-03
83	.5401726D+01	.6304441D-03	.7632052D-03	.5554688D-03	.1100917D-03	.1000000D-08	.1271761D-04	.3554397D-03
84	.5466807D+01	.6281951D-03	.7616987D-03	.5544439D-03	.1096067D-03	.1000000D-08	.1269415D-04	.3534727D-03
85	.5531888D+01	.6259520D-03	.7601940D-03	.5534198D-03	.1091236D-03	.1000000D-08	.1267070D-04	.3515147D-03
86	.5596969D+01	.6237145D-03	.7586910D-03	.5523968D-03	.1086425D-03	.1000000D-08	.1264728D-04	.3495658D-03
87	.5662050D+01	.6214835D-03	.7571897D-03	.5513749D-03	.1081634D-03	.1000000D-08	.1262388D-04	.3476261D-03
88	.5727131D+01	.6192587D-03	.7556902D-03	.5503542D-03	.1076862D-03	.1000000D-08	.1260051D-04	.3456957D-03
89	.5792212D+01	.6170386D-03	.7541930D-03	.5493348D-03	.1072110D-03	.1000000D-08	.1257717D-04	.3437739D-03
90	.5857293D+01	.6148244D-03	.7526978D-03	.5483169D-03	.1067376D-03	.1000000D-08	.1255387D-04	.3418612D-03
91	.5922374D+01	.6126156D-03	.7512050D-03	.5473006D-03	.1062662D-03	.1000000D-08	.1253060D-04	.3399574D-03
92	.5987455D+01	.6104106D-03	.7497140D-03	.5462862D-03	.1057967D-03	.1000000D-08	.1250738D-04	.3380621D-03
93	.6052536D+01	.6082111D-03	.7482278D-03	.5452737D-03	.1053291D-03	.1000000D-08	.1248419D-04	.3361757D-03
94	.6117617D+01	.6060169D-03	.7467431D-03	.5442634D-03	.1048634D-03	.1000000D-08	.1246106D-04	.3342982D-03
95	.6182698D+01	.6038266D-03	.7452618D-03	.5432554D-03	.1043995D-03	.1000000D-08	.1243798D-04	.3324292D-03
96	.6247779D+01	.6016409D-03	.7437836D-03	.5422500D-03	.1039375D-03	.1000000D-08	.1241497D-04	.3305689D-03
97	.6312860D+01	.5994599D-03	.7423088D-03	.5412474D-03	.1034774D-03	.1000000D-08	.1239201D-04	.3287175D-03
98	.6377941D+01	.5972825D-03	.7408377D-03	.5402478D-03	.1030191D-03	.1000000D-08	.1236912D-04	.3268745D-03
99	.6443022D+01	.5921409D-03	.7404975D-03	.5392508D-03	.1025624D-03	.1000000D-08	.1234630D-04	.3239118D-03
100	.6508103D+01	.5899893D-03	.7390235D-03	.5382550D-03	.1021075D-03	.1000000D-08	.1232350D-04	.3220924D-03
101	.6573184D+01	.5878433D-03	.7375514D-03	.5372605D-03	.1016544D-03	.1000000D-08	.1230073D-04	.3202816D-03
102	.6638265D+01	.5857024D-03	.7360814D-03	.5362673D-03	.1012030D-03	.1000000D-08	.1227799D-04	.3184791D-03
103	.6703346D+01	.5835672D-03	.7346131D-03	.5352752D-03	.1007535D-03	.1000000D-08	.1225527D-04	.3166851D-03
104	.6768427D+01	.5814382D-03	.7331464D-03	.5342842D-03	.1003059D-03	.1000000D-08	.1223259D-04	.3148998D-03
105	.6833508D+01	.5793154D-03	.7316813D-03	.5332944D-03	.9986002D-04	.1000000D-08	.1220992D-04	.3131231D-03
106	.6898589D+01	.5771987D-03	.7302177D-03	.5323055D-03	.9941596D-04	.1000000D-08	.1218728D-04	.3113550D-03
107	.6963670D+01	.5750877D-03	.7287557D-03	.5313179D-03	.9897369D-04	.1000000D-08	.1216467D-04	.3095952D-03
108	.7028751D+01	.5729821D-03	.7272955D-03	.5303311D-03	.9853318D-04	.1000000D-08	.1214208D-04	.3078435D-03
109	.7093832D+01	.5708816D-03	.7258372D-03	.5293454D-03	.9809446D-04	.1000000D-08	.1211951D-04	.3061001D-03
110	.7158914D+01	.5687873D-03	.7243804D-03	.5283609D-03	.9765751D-04	.1000000D-08	.1209697D-04	.3043650D-03
111	.7223995D+01	.5666993D-03	.7229252D-03	.5273775D-03	.9722233D-04	.1000000D-08	.1207445D-04	.3026383D-03
112	.7289076D+01	.5646168D-03	.7214716D-03	.5263952D-03	.9678891D-04	.1000000D-08	.1205196D-04	.3009201D-03
113	.7354157D+01	.5625405D-03	.7200197D-03	.5254141D-03	.9635724D-04	.1000000D-08	.1202950D-04	.2992101D-03
114	.7419238D+01	.5604731D-03	.7185694D-03	.5244342D-03	.9592731D-04	.1000000D-08	.1200707D-04	.2975084D-03
115	.7484319D+01	.5584055D-03	.7171210D-03	.5234557D-03	.9549912D-04	.1000000D-08	.1198466D-04	.2958150D-03
116	.7549400D+01	.5563467D-03	.7156743D-03	.5224785D-03	.9507266D-04	.1000000D-08	.1196229D-04	.2941298D-03
117	.7614481D+01	.5542921D-03	.7142297D-03	.5215028D-03	.9464792D-04	.1000000D-08	.1193995D-04	.2924526D-03
118	.7679562D+01	.5522435D-03	.7127877D-03	.5205288D-03	.9422488D-04	.1000000D-08	.1191765D-04	.2907829D-03
119	.7744643D+01	.5501997D-03	.7113478D-03	.5195563D-03	.9380346D-04	.1000000D-08	.1189539D-04	.2891213D-03
120	.7809724D+01	.5481603D-03	.7099100D-03	.5185856D-03	.9338378D-04	.1000000D-08	.1187316D-04	.2874677D-03
121	.7874805D+01	.5461267D-03	.7084746D-03	.5176167D-03	.9296579D-04	.1000000D-08	.1185098D-04	.2858221D-03
122	.7939886D+01	.5440993D-03	.7070415D-03	.5166497D-03	.9254947D-04	.1000000D-08	.1182884D-04	.2841845D-03
123	.8004967D+01	.5420749D-03	.7056108D-03	.5156847D-03	.9213483D-04	.1000000D-08	.1180675D-04	.2825548D-03
124	.8070048D+01	.5400565D-03	.7041828D-03	.5147219D-03	.9172185D-04	.1000000D-08	.1178470D-04	.2809330D-03
125	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	.1000000D-08	[illegible]	[illegible]
126	.8200210D+01	.5360331D-03	.7013355D-03	.5128032D-03	.9090084D-04	.1000000D-08	.1174077D-04	.2777126D-03
127	.8265291D+01	.5340279D-03	.6999165D-03	.5118475D-03	.9049280D-04	.1000000D-08	.1171889D-04	.2761139D-03
128	.8330372D+01	.5320271D-03	.6985006D-03	.5108945D-03	.9008638D-04	.1000000D-08	.1169707D-04	.2745229D-03
129	.8395453D+01	.5274556D-03	.6980413D-03	.5099434D-03	.8968155D-04	.1000000D-08	.1167530D-04	.2719851D-03
130	.8460534D+01	.5254824D-03	.6966180D-03	.5089895D-03	.8927812D-04	.1000000D-08	.1165346D-04	.2704156D-03
131	.8525615D+01	.5235167D-03	.6951964D-03	.5080370D-03	.8887632D-04	.1000000D-08	.1163165D-04	.2688538D-03
132	.8590696D+01	.5215556D-03	.6937767D-03	.5070859D-03	.8847613D-04	.1000000D-08	.1160987D-04	.2672997D-03

133	.8655777D+01	.5196001D-03	.6923587D-03	.5061360D-03	.8807754D-04	.1000000D-08	.1158812D-04	.2657532D-03
134	.8720858D+01	.5176494D-03	.6909426D-03	.5051874D-03	.8768056D-04	.1000000D-08	.1156641D-04	.2642140D-03
135	.8785939D+01	.5157042D-03	.6895283D-03	.5042400D-03	.8728518D-04	.1000000D-08	.1154472D-04	.2626823D-03
136	.8851020D+01	.5137646D-03	.6881156D-03	.5032938D-03	.8689139D-04	.1000000D-08	.1152305D-04	.2611582D-03
137	.8916101D+01	.5118307D-03	.6867044D-03	.5023487D-03	.8649918D-04	.1000000D-08	.1150141D-04	.2596416D-03
138	.8981182D+01	.5099023D-03	.6852949D-03	.5014049D-03	.8610854D-04	.1000000D-08	.1147980D-04	.2581325D-03
139	.9046263D+01	.5079796D-03	.6838870D-03	.5004621D-03	.8571948D-04	.1000000D-08	.1145822D-04	.2566308D-03
140	.9111344D+01	.5060625D-03	.6824806D-03	.4995206D-03	.8533198D-04	.1000000D-08	.1143666D-04	.2551365D-03
141	.9176425D+01	.5041510D-03	.6810758D-03	.4985802D-03	.8494603D-04	.1000000D-08	.1141513D-04	.2536496D-03
142	.9241507D+01	.5022442D-03	.6796730D-03	.4976410D-03	.8456164D-04	.1000000D-08	.1139363D-04	.2521698D-03
143	.9306588D+01	.5003429D-03	.6782718D-03	.4967030D-03	.8417879D-04	.1000000D-08	.1137215D-04	.2506973D-03
144	.9371669D+01	.4984470D-03	.6768723D-03	.4957662D-03	.8379748D-04	.1000000D-08	.1135071D-04	.2492320D-03
145	.9436750D+01	.4965567D-03	.6754744D-03	.4948306D-03	.8341769D-04	.1000000D-08	.1132929D-04	.2477740D-03
146	.9501831D+01	.4946717D-03	.6740782D-03	.4938964D-03	.8303944D-04	.1000000D-08	.1130790D-04	.2463233D-03
147	.9566912D+01	.4927921D-03	.6726837D-03	.4929634D-03	.8266270D-04	.1000000D-08	.1128653D-04	.2448797D-03
148	.9631993D+01	.4909178D-03	.6712911D-03	.4920318D-03	.8228746D-04	.1000000D-08	.1126521D-04	.2434432D-03
149	.9697074D+01	.4890486D-03	.6699003D-03	.4911016D-03	.8191374D-04	.1000000D-08	.1124391D-04	.2420139D-03
150	.9762155D+01	.4871839D-03	.6685116D-03	.4901728D-03	.8154151D-04	.1000000D-08	.1122264D-04	.2405914D-03
151	.9827236D+01	.4853245D-03	.6671249D-03	.4892455D-03	.8117077D-04	.1000000D-08	.1120141D-04	.2391759D-03
152	.9892317D+01	.4834701D-03	.6657401D-03	.4883198D-03	.8080151D-04	.1000000D-08	.1118022D-04	.2377674D-03
153	.9957398D+01	.4816207D-03	.6643573D-03	.4873956D-03	.8043373D-04	.1000000D-08	.1115906D-04	.2363660D-03
154	.1002248D+02	.4797764D-03	.6629766D-03	.4864730D-03	.8006742D-04	.1000000D-08	.1113794D-04	.2349715D-03

FOR51

DAT

File: DSKB:FOR51.DAT[6452,232] Created: 07-Oct-84 16:55:00 <055> Printed: 07-Oct-84 16:56:54
QUEUE Switches: /FILE:FORT /COPIES:1 /SPACING:1 /LIMIT:273

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0.6508103D-01	0.4922630D-02	0.1000000D-04	0.4922630D-02
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0.1952431D+00	0.4891340D-02	0.9927465D-05	0.1472093D-01
0.2603241D+00	0.4875771D-02	0.9891371D-05	0.1959670D-01
0.3254052D+00	0.4860251D-02	0.9855392D-05	0.2445695D-01
0.3904862D+00	0.4844781D-02	0.9819527D-05	0.2930173D-01
0.4555672D+00	0.4829361D-02	0.9783776D-05	0.3413109D-01
0.5206482D+00	0.4813990D-02	0.9748139D-05	0.3894508D-01
0.5857293D+00	0.4798669D-02	0.9712616D-05	0.4374375D-01
0.6508103D+00	0.4783395D-02	0.9677206D-05	0.4852715D-01
0.7158914D+00	0.4768169D-02	0.9641908D-05	0.5329532D-01
0.7809724D+00	0.4752988D-02	0.9606723D-05	0.5804830D-01
0.8460534D+00	0.4737856D-02	0.9571649D-05	0.6278616D-01
0.9111344D+00	0.4722772D-02	0.9536688D-05	0.6750893D-01
0.9762155D+00	0.4707736D-02	0.9501837D-05	0.7221667D-01
0.1041297D+01	0.4692748D-02	0.9467098D-05	0.7690942D-01
0.1106378D+01	0.4677808D-02	0.9432469D-05	0.8158723D-01
0.1171459D+01	0.4662916D-02	0.9397951D-05	0.8625014D-01
0.1236540D+01	0.4648070D-02	0.9363542D-05	0.9089821D-01
0.1301621D+01	0.4633273D-02	0.9329243D-05	0.9553148D-01
0.1366702D+01	0.4618522D-02	0.9295053D-05	0.1001500D+00
0.1431783D+01	0.4603818D-02	0.9260572D-05	0.1047538D+00
0.1496864D+01	0.4589161D-02	0.9226999D-05	0.1093430D+00
0.1561945D+01	0.4574550D-02	0.9193135D-05	0.1139175D+00
0.1627026D+01	0.4559986D-02	0.9159378D-05	0.1184775D+00
0.1692107D+01	0.4545468D-02	0.9125729D-05	0.1230230D+00
0.1757188D+01	0.4530996D-02	0.9092187D-05	0.1275540D+00
0.1822269D+01	0.4516570D-02	0.9058752D-05	0.1320706D+00
0.1887350D+01	0.4502190D-02	0.9025424D-05	0.1365727D+00
0.1952431D+01	0.4487855D-02	0.8992201D-05	0.1410606D+00
0.2017512D+01	0.4473563D-02	0.8959084D-05	0.1455342D+00
0.2082593D+01	0.4459314D-02	0.8926073D-05	0.1499935D+00
0.2147674D+01	0.4445111D-02	0.8893166D-05	0.1544386D+00
0.2212755D+01	0.4430952D-02	0.8860365D-05	0.1588695D+00
0.2277836D+01	0.4416838D-02	0.8827668D-05	0.1632864D+00
0.2342917D+01	0.4402769D-02	0.8795075D-05	0.1676891D+00
0.2407998D+01	0.4388744D-02	0.8762586D-05	0.1720779D+00
0.2473079D+01	0.4374764D-02	0.8730201D-05	0.1764527D+00
0.2538160D+01	0.4360828D-02	0.8697919D-05	0.1808135D+00
0.2603241D+01	0.4346935D-02	0.8665739D-05	0.1851604D+00
0.2668322D+01	0.4333087D-02	0.8633662D-05	0.1894935D+00
0.2733403D+01	0.4319282D-02	0.8601687D-05	0.1938128D+00
0.2798484D+01	0.4305521D-02	0.8569815D-05	0.1981183D+00
0.2863565D+01	0.4291803D-02	0.8538043D-05	0.2024101D+00
0.2928646D+01	0.4278128D-02	0.8506373D-05	0.2066882D+00
0.2993727D+01	0.4264496D-02	0.8474804D-05	0.2109527D+00
0.3059808D+01	0.4250907D-02	0.8443335D-05	0.2152036D+00
0.3123890D+01	0.4237361D-02	0.8411967D-05	0.2194410D+00
0.3188971D+01	0.4223857D-02	0.8380699D-05	0.2236649D+00
0.3254052D+01	0.4210396D-02	0.8349530D-05	0.2278753D+00
0.3319133D+01	0.4196977D-02	0.8318460D-05	0.2320722D+00
0.3384214D+01	0.4183598D-02	0.8287490D-05	0.2362558D+00
0.3449295D+01	0.4170259D-02	0.8256618D-05	0.2404261D+00
0.3514376D+01	0.4156962D-02	0.8225845D-05	0.2445831D+00
0.3579457D+01	0.4143707D-02	0.8195170D-05	0.2487268D+00
0.3644538D+01	0.4130497D-02	0.8164593D-05	0.2528573D+00
0.3709619D+01	0.4117321D-02	0.8134113D-05	0.2569746D+00
0.3774700D+01	0.4104190D-02	0.8103730D-05	0.2610788D+00
0.3839781D+01	0.4091107D-02	0.8073445D-05	0.2651699D+00
0.3904862D+01	0.4078051D-02	0.8043256D-05	0.2692479D+00
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0.4035024D+01	0.4052075D-02	0.7983166D-05	0.2773650D+00
0.4100105D+01	0.4039148D-02	0.7953265D-05	0.2814042D+00
0.4165186D+01	0.4026262D-02	0.7923459D-05	0.2854204D+00
0.4230267D+01	0.4013415D-02	0.7893743D-05	0.2894439D+00
0.4295348D+01	0.4000609D-02	0.7864133D-05	0.2934445D+00
0.4360429D+01	0.3987843D-02	0.7834611D-05	0.2974323D+00
0.4425510D+01	0.3975116D-02	0.7805184D-05	0.3014074D+00
0.4490591D+01	0.3962429D-02	0.7775851D-05	0.3053699D+00
0.4555672D+01	0.3949782D-02	0.7746611D-05	0.3093196D+00
0.4620753D+01	0.3937174D-02	0.7717465D-05	0.3132568D+00
0.4685834D+01	0.3924605D-02	0.7688412D-05	0.3171814D+00
0.4750915D+01	0.3912076D-02	0.7659451D-05	0.3210935D+00
0.4815996D+01	0.3899583D-02	0.7630583D-05	0.3249931D+00
0.4881077D+01	0.3887128D-02	0.7601808D-05	0.3288802D+00
0.4946158D+01	0.3874711D-02	0.7573124D-05	0.3327549D+00
0.5011239D+01	0.3862333D-02	0.7544531D-05	0.3366172D+00
0.5076320D+01	0.3849994D-02	0.7516030D-05	0.3404672D+00
0.5141402D+01	0.3837693D-02	0.7487620D-05	0.3443049D+00
0.5206483D+01	0.3825430D-02	0.7459301D-05	0.3481304D+00
0.5271564D+01	0.3813205D-02	0.7431073D-05	0.3519436D+00
0.5336645D+01	0.3801018D-02	0.7402934D-05	0.3557446D+00
0.5401726D+01	0.3788868D-02	0.7374886D-05	0.3595335D+00
0.5466807D+01	0.3776757D-02	0.7346927D-05	0.3633102D+00
0.5531888D+01	0.3764682D-02	0.7319057D-05	0.3670749D+00
0.5596969D+01	0.3752645D-02	0.7291277D-05	0.3708275D+00
0.5662050D+01	0.3740646D-02	0.7263585D-05	0.3745682D+00
0.5727131D+01	0.3728683D-02	0.7235982D-05	0.3782969D+00
0.5792212D+01	0.3716758D-02	0.7208468D-05	0.3820136D+00
0.5857293D+01	0.3704869D-02	0.7181041D-05	0.3857185D+00
0.5922374D+01	0.3693017D-02	0.7153702D-05	0.3894115D+00
0.5987455D+01	0.3681201D-02	0.7126450D-05	0.3930927D+00
0.6052536D+01	0.3669422D-02	0.7099286D-05	0.3967621D+00
0.6117617D+01	0.3657679D-02	0.7072209D-05	0.4004198D+00
0.6182698D+01	0.3645972D-02	0.7045218D-05	0.4040658D+00
0.6247779D+01	0.3634301D-02	0.7018313D-05	0.4077001D+00
0.6312860D+01	0.3622666D-02	0.6991495D-05	0.4113228D+00

0.6377941D+01	0.3611067D-02	0.6964763D-05	0.4149338D+00
0.6443022D+01	0.3599503D-02	0.6938116D-05	0.4185333D+00
0.6508103D+01	0.3587972D-02	0.6911554D-05	0.4221213D+00
0.6573184D+01	0.3576477D-02	0.6885078D-05	0.4256978D+00
0.6638265D+01	0.3565017D-02	0.6858686D-05	0.4292628D+00
0.6703346D+01	0.3553592D-02	0.6832379D-05	0.4328164D+00
0.6768427D+01	0.3542203D-02	0.6806157D-05	0.4363586D+00
0.6833508D+01	0.3530848D-02	0.6780018D-05	0.4398894D+00
0.6898589D+01	0.[illegible]19529D-02	0.6753963D-05	0.4434090D+00
0.6963670D+01	0.3508244D-02	0.6727992D-05	0.4469172D+00
0.7028751D+01	0.3496993D-02	0.6702104D-05	0.4504142D+00
0.7093832D+01	0.3485777D-02	0.6676299D-05	0.4539000D+00
0.7158914D+01	0.3474595D-02	0.6650576D-05	0.4573746D+00
0.7223995D+01	0.3463448D-02	0.6624937D-05	0.4608380D+00
0.7289076D+01	0.3452335D-02	0.6599379D-05	0.4642904D+00
0.7354157D+01	0.3441255D-02	0.6573904D-05	0.4677316D+00
0.7419238D+01	0.3430210D-02	0.6548510D-05	0.4711618D+00
0.7484319D+01	0.3419198D-02	0.6523198D-05	0.4745810D+00
0.7549400D+01	0.3408220D-02	0.6497967D-05	0.4779892D+00
0.7614481D+01	0.3397276D-02	0.6472817D-05	0.4813865D+00
0.7679562D+01	0.3386365D-02	0.6447747D-05	0.4847729D+00
0.7744643D+01	0.3375487D-02	0.6422759D-05	0.4881484D+00
0.7809724D+01	0.3364642D-02	0.6397850D-05	0.4915130D+00
0.7874805D+01	0.3353830D-02	0.6373022D-05	0.4948668D+00
0.7939886D+01	0.3343051D-02	0.6348273D-05	0.4982099D+00
0.8004967D+01	0.3332305D-02	0.6323604D-05	0.5015422D+00
0.8070048D+01	0.3321592D-02	0.6299014D-05	0.5048638D+00
0.8135129D+01	0.3310912D-02	0.6274504D-05	0.5081747D+00
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0.8330372D+01	0.3279064D-02	0.6201443D-05	0.5180437D+00
0.8395453D+01	0.3268513D-02	0.6177246D-05	0.5213122D+00
0.8460534D+01	0.3257991D-02	0.6153127D-05	0.5245702D+00
0.8525615D+01	0.3247502D-02	0.6129066D-05	0.5278177D+00
0.8590696D+01	0.3237044D-02	0.6105122D-05	0.5310547D+00
0.8655777D+01	0.3226619D-02	0.6081235D-05	0.5342813D+00
0.8720858D+01	0.3216225D-02	0.6057425D-05	0.5374976D+00
0.8785939D+01	0.3205362D-02	0.6033692D-05	0.5407034D+00
0.8851020D+01	0.3195531D-02	0.6010035D-05	0.5438990D+00
0.8916101D+01	0.3185231D-02	0.5986455D-05	0.5470842D+00
0.8981182D+01	0.3174963D-02	0.5962550D-05	0.5502592D+00
0.9046263D+01	0.3164726D-02	0.5939522D-05	0.5534239D+00
0.9111344D+01	0.3154519D-02	0.5916168D-05	0.5565784D+00
0.9176425D+01	0.3144344D-02	0.5892891D-05	0.5597227D+00
0.9241507D+01	0.3134199D-02	0.5869688D-05	0.5628569D+00
0.9306588D+01	0.3124085D-02	0.5846560D-05	0.5659810D+00
0.9371669D+01	0.3114002D-02	0.5823507D-05	0.5690950D+00
0.9436750D+01	0.3103949D-02	0.5800528D-05	0.5721990D+00
0.9501831D+01	0.3093926D-02	0.5777623D-05	0.5752929D+00
0.9566912D+01	0.3083934D-02	0.5754792D-05	0.5783768D+00
0.9631993D+01	0.3073972D-02	0.5732035D-05	0.5814508D+00
0.9697074D+01	0.3064039D-02	0.5709352D-05	0.5845148D+00
0.9762155D+01	0.3054137D-02	0.5686742D-05	0.5875690D+00
0.9827236D+01	0.3044265D-02	0.5664204D-05	0.5906132D+00
0.9892317D+01	0.3034422D-02	0.5641740D-05	0.5936477D+00
0.9957398D+01	0.3024609D-02	0.5619349D-05	0.5966723D+00
0.1002248D+02	0.3014826D-02	0.5597029D-05	0.5996871D+00

FOR52

DAT

File: DSKB:FOR52.DAT[6452,232] Created: 07-Oct-84 16:55:00 <055> Printed: 07-Oct-84 16:56:55
QUEUE Switches: /FILE:FORT /COPIES:1 /SPACING:1 /LIMIT:270

CONCENTRATION OF THE SPRAYED SOLUTION IN THE SUMP

#	TIME	I2	I-	HOI	IO3-	H+	IO-	I3-
1	.6508133D-01	.8540259D-03	.8872849D-03	.6453274D-03	.1573912D-03	.1000000D-08	.1477495D-04	.5597734D-03
2	.1301621D+00	.7322797D-03	.9984260D-03	.5453664D-03	.2040027D-03	.1000000D-08	.1248632D-04	.5794403D-03
3	.1952431D+00	.7484437D-03	.1079732D-02	.4820146D-03	.2352856D-03	.1000000D-08	.1103586D-04	.5897461D-03
4	.2603241D+00	.7147184D-03	.1143780D-02	.4373645D-03	.2583611D-03	.1000000D-08	.1001358D-04	.5954435D-03
5	.3254052D+00	.6874515D-03	.1196448D-02	.4037016D-03	.2764084D-03	.1000000D-08	.9242861D-05	.5985383D-03
6	.3904862D+00	.6646304D-03	.1241217D-02	.3771351D-03	.2910942D-03	.1000000D-08	.8634614D-05	.6000233D-03
7	.4555672D+00	.6450341D-03	.1280117D-02	.3554731D-03	.3033903D-03	.1000000D-08	.8138656D-05	.6004459D-03
8	.5206483D+00	.6279058D-03	.1314455D-02	.3373302D-03	.3139089D-03	.1000000D-08	.7723270D-05	.6001432D-03
9	.5857293D+00	.6126946D-03	.1345188D-02	.3218485D-03	.3230580D-03	.1000000D-08	.7368812D-05	.5993196D-03
10	.6508103D+00	.5990257D-03	.1372979D-02	.3084213D-03	.3311225D-03	.1000000D-08	.7061392D-05	.5981160D-03
11	.7158914D+00	.5962139D-03	.1398458D-02	.2966319D-03	.3383082D-03	.1000000D-08	.6791470D-05	.5964665D-03
12	.7809724D+00	.5747145D-03	.1421784D-02	.2860647D-03	.3447515D-03	.1000000D-08	.6549531D-05	.5945874D-03
13	.8460534D+00	.5641492D-03	.1443261D-02	.2766101D-03	.3505777D-03	.1000000D-08	.6333066D-05	.5925707D-03
14	.9111344D+00	.5543678D-03	.1463158D-02	.2680893D-03	.3558832D-03	.1000000D-08	.6137980D-05	.5904451D-03
15	.9762155D+00	.5452672D-03	.1481784D-02	.2603429D-03	.3607436D-03	.1000000D-08	.5960624D-05	.5882379D-03
16	.1041247D+01	.5367581D-03	.1499181D-02	.2532563D-03	.3652188D-03	.1000000D-08	.5798374D-05	.5859675D-03
17	.1106378D+01	.5287610D-03	.1515538D-02	.2467463D-03	.3693575D-03	.1000000D-08	.5649326D-05	.5836456D-03
18	.1171459D+01	.5212238D-03	.1530950D-02	.2407272D-03	.3731994D-03	.1000000D-08	.5511517D-05	.5812868D-03
19	.1236540D+01	.5140955D-03	.1545515D-02	.2351391D-03	.3767785D-03	.1000000D-08	.5383575D-05	.5788999D-03
20	.1301621D+01	.5073347D-03	.1559311D-02	.2299289D-03	.3801221D-03	.1000000D-08	.5264287D-05	.5764926D-03
21	.1366702D+01	.5008956D-03	.1572426D-02	.2250681D-03	.3832542D-03	.1000000D-08	.5152997D-05	.5740664D-03
22	.1431783D+01	.4947586D-03	.1584897D-02	.2205035D-03	.3861953D-03	.1000000D-08	.5048489D-05	.5716314D-03
23	.1496864D+01	.4888965D-03	.1596778D-02	.2162046D-03	.3889630D-03	.1000000D-08	.4950065D-05	.5691915D-03
24	.1561945D+01	.4832808D-03	.1608125D-02	.2121526D-03	.3915725D-03	.1000000D-08	.4857294D-05	.5667473D-03
25	.1627026D+01	.4778867D-03	.1618987D-02	.2083305D-03	.3940372D-03	.1000000D-08	.4769786D-05	.5642996D-03
26	.1692107D+01	.4727049D-03	.1629382D-02	.2047053D-03	.3963689D-03	.1000000D-08	.4686784D-05	.5618548D-03
27	.1757188D+01	.4677189D-03	.1639343D-02	.2012600D-03	.3985789D-03	.1000000D-08	.4607903D-05	.5594147D-03
28	.1822269D+01	.4629131D-03	.1648903D-02	.1979813D-03	.4006737D-03	.1000000D-08	.4532836D-05	.5569802D-03
29	.1887350D+01	.4582706D-03	.1658094D-02	.1948618D-03	.4026643D-03	.1000000D-08	.4461416D-05	.5545503D-03
30	.1952431D+01	.4537866D-03	.1666928D-02	.1918792D-03	.4045571D-03	.1000000D-08	.4393129D-05	.5521298D-03

31	.2017512D+01	.4493165D-03	.1675485D-02	.1890289D-03	.4063588D-03	.1000000D-08	.4327870D-05	.5496658D-03
32	.2082593D+01	.4450510D-03	.1683707D-02	.1862742D-03	.4080719D-03	.1000000D-08	.4264801D-05	.5471910D-03
33	.2147674D+01	.4409177D-03	.1691630D-02	.1836423D-03	.4097026D-03	.1000000D-08	.4204543D-05	.5447298D-03
34	.2212755D+01	.4369115D-03	.1699264D-02	.1811184D-03	.4112567D-03	.1000000D-08	.4146756D-05	.5422843D-03
35	.2277836D+01	.4330258D-03	.1706623D-02	.1786921D-03	.4127390D-03	.1000000D-08	.4091206D-05	.5398552D-03
36	.2342917D+01	.4292516D-03	.1713726D-02	.1763593D-03	.4141541D-03	.1000000D-08	.4037796D-05	.5374416D-03
37	.2407998D+01	.4255619D-03	.1720587D-02	.1741140D-03	.4155060D-03	.1000000D-08	.3986388D-05	.5350432D-03
38	.2473079D+01	.4220108D-03	.1727220D-02	.1719503D-03	.4167986D-03	.1000000D-08	.3936849D-05	.5326599D-03
39	.2538160D+01	.4185327D-03	.1733636D-02	.1698631D-03	.4180350D-03	.1000000D-08	.3889062D-05	.5302917D-03
40	.2603241D+01	.4151426D-03	.1739845D-02	.1678477D-03	.4192185D-03	.1000000D-08	.3842921D-05	.5279383D-03
41	.2668322D+01	.4118359D-03	.1745858D-02	.1659000D-03	.4203519D-03	.1000000D-08	.3798328D-05	.5255996D-03
42	.2733403D+01	.4086101D-03	.1751680D-02	.1640129D-03	.4214378D-03	.1000000D-08	.3755121D-05	.5232768D-03
43	.2798484D+01	.4054570D-03	.1757329D-02	.1621899D-03	.4224786D-03	.1000000D-08	.3713382D-05	.5209658D-03
44	.2863565D+01	.4023751D-03	.1762808D-02	.1604241D-03	.4234765D-03	.1000000D-08	.3672953D-05	.5186710D-03
45	.2928646D+01	.3993603D-03	.1768127D-02	.1587138D-03	.4244335D-03	.1000000D-08	.3633797D-05	.5163886D-03
46	.2993727D+01	.3964174D-03	.1773289D-02	.1570546D-03	.4253517D-03	.1000000D-08	.3595808D-05	.5141202D-03
47	.3058808D+01	.3935230D-03	.1778300D-02	.1554430D-03	.4262327D-03	.1000000D-08	.3558911D-05	.5118660D-03
48	.3123890D+01	.3906954D-03	.1783166D-02	.1538768D-03	.4270783D-03	.1000000D-08	.3523052D-05	.5096257D-03
49	.3188971D+01	.3879248D-03	.1787893D-02	.1523539D-03	.4278901D-03	.1000000D-08	.3488184D-05	.5073992D-03
50	.3254052D+01	.3852090D-03	.1792487D-02	.1508721D-03	.4286693D-03	.1000000D-08	.3454260D-05	.5051863D-03
51	.3319133D+01	.3825455D-03	.1796952D-02	.1494298D-03	.4294175D-03	.1000000D-08	.3421236D-05	.5029868D-03
52	.3384214D+01	.3798616D-03	.1801321D-02	.1480251D-03	.4301359D-03	.1000000D-08	.3389077D-05	.5007729D-03
53	.3449295D+01	.3772630D-03	.1805562D-02	.1466418D-03	.4308243D-03	.1000000D-08	.3357405D-05	.4985584D-03
54	.3514376D+01	.3747147D-03	.1809682D-02	.1452946D-03	.4314840D-03	.1000000D-08	.3326559D-05	.4963593D-03
55	.3579457D+01	.3722131D-03	.1813684D-02	.1439817D-03	.4321163D-03	.1000000D-08	.3296502D-05	.4941753D-03
56	.3644538D+01	.3697577D-03	.1817574D-02	.1427017D-03	.4327223D-03	.1000000D-08	.3267195D-05	.4920061D-03
57	.3709619D+01	.3673462D-03	.1821357D-02	.1414530D-03	.4333033D-03	.1000000D-08	.3238606D-05	.4898513D-03
58	.3774700D+01	.3649770D-03	.1825034D-02	.1402339D-03	.4338601D-03	.1000000D-08	.3210694D-05	.4877109D-03
59	.3839781D+01	.3626481D-03	.1828612D-02	.1390438D-03	.4343937D-03	.1000000D-08	.3183446D-05	.4855842D-03
60	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
61	.3969943D+01	.3581059D-03	.1835480D-02	.1367447D-03	.4353951D-03	.1000000D-08	.3130809D-05	.4813716D-03
62	.4035024D+01	.3558879D-03	.1838776D-02	.1356336D-03	.4358645D-03	.1000000D-08	.3105369D-05	.4792852D-03
63	.4100105D+01	.3527089D-03	.1841985D-02	.1345467D-03	.4363140D-03	.1000000D-08	.3080484D-05	.4772119D-03
64	.4165186D+01	.3515617D-03	.1845110D-02	.1334831D-03	.4367444D-03	.1000000D-08	.3056133D-05	.4751513D-03
65	.4230267D+01	.3494471D-03	.1848152D-02	.1324419D-03	.4371562D-03	.1000000D-08	.3032295D-05	.4731033D-03
66	.4295348D+01	.3473642D-03	.1851115D-02	.1314223D-03	.4375502D-03	.1000000D-08	.3008950D-05	.4710678D-03
67	.4360429D+01	.3453119D-03	.1854000D-02	.1304234D-03	.4379270D-03	.1000000D-08	.2986081D-05	.4690445D-03
68	.4425510D+01	.3432892D-03	.1856810D-02	.1294446D-03	.4382870D-03	.1000000D-08	.2963671D-05	.4670333D-03
69	.4490591D+01	.3412952D-03	.1859548D-02	.1284851D-03	.4386309D-03	.1000000D-08	.2941702D-05	.4650339D-03
70	.4555672D+01	.3393292D-03	.1862214D-02	.1275442D-03	.4389592D-03	.1000000D-08	.2920161D-05	.4630463D-03
71	.4620753D+01	.3373901D-03	.1864812D-02	.1266214D-03	.4392724D-03	.1000000D-08	.2899031D-05	.4610703D-03
72	.4685834D+01	.3354773D-03	.1867343D-02	.1257159D-03	.4395708D-03	.1000000D-08	.2878300D-05	.4591057D-03
73	.4750915D+01	.3335899D-03	.1869808D-02	.1248272D-03	.4398551D-03	.1000000D-08	.2857954D-05	.4571524D-03
74	.4815996D+01	.3316923D-03	.1872228D-02	.1239548D-03	.4401256D-03	.1000000D-08	.2837980D-05	.4551928D-03
75	.4881077D+01	.3298222D-03	.1874583D-02	.1230891D-03	.4403819D-03	.1000000D-08	.2818160D-05	.4532343D-03
76	.4946158D+01	.3279871D-03	.1876874D-02	.1222396D-03	.4406246D-03	.1000000D-08	.2798709D-05	.4512878D-03
77	.5011239D+01	.3261763D-03	.1879102D-02	.1214055D-03	.4408541D-03	.1000000D-08	.2779612D-05	.4493534D-03
78	.5076320D+01	.3243891D-03	.1881271D-02	.1205863D-03	.4410709D-03	.1000000D-08	.2760858D-05	.4474308D-03
79	.5141402D+01	.3226248D-03	.1883381D-02	.1197816D-03	.4412753D-03	.1000000D-08	.2742434D-05	.4455197D-03
80	.5206483D+01	.3208828D-03	.1885434D-02	.1189909D-03	.4414678D-03	.1000000D-08	.2724330D-05	.4436200D-03
81	.5271564D+01	.3191624D-03	.1887432D-02	.1182137D-03	.4416486D-03	.1000000D-08	.2706536D-05	.4417315D-03
82	.5336645D+01	.3174630D-03	.1889375D-02	.1174960D-03	.4418182D-03	.1000000D-08	.2689041D-05	.4398541D-03
83	.5401726D+01	.3157840D-03	.1891267D-02	.1166981D-03	.4419769D-03	.1000000D-08	.2671837D-05	.4379876D-03
84	.5466807D+01	.3141250D-03	.1893107D-02	.1159590D-03	.4421249D-03	.1000000D-08	.2654913D-05	.4361318D-03
85	.5531888D+01	.3124853D-03	.1894897D-02	.1152317D-03	.4422627D-03	.1000000D-08	.2638262D-05	.4342866D-03
86	.5596969D+01	.3108645D-03	.1896638D-02	.1145160D-03	.4423904D-03	.1000000D-08	.2621876D-05	.4324518D-03
87	.5662050D+01	.3092622D-03	.1898332D-02	.1138115D-03	.4425085D-03	.1000000D-08	.2605747D-05	.4306273D-03
88	.5727131D+01	.3076778D-03	.1899980D-02	.1131179D-03	.4426170D-03	.1000000D-08	.2589867D-05	.4288129D-03
89	.5792212D+01	.3061109D-03	.1901582D-02	.1124349D-03	.4427164D-03	.1000000D-08	.2574229D-05	.4270086D-03
90	.5857293D+01	.3045611D-03	.1903140D-02	.1117622D-03	.4428067D-03	.1000000D-08	.2558827D-05	.4252143D-03
91	.5922374D+01	.3030280D-03	.1904655D-02	.1110995D-03	.4428884D-03	.1000000D-08	.2543654D-05	.4234297D-03
92	.5987455D+01	.3015111D-03	.1906128D-02	.1104465D-03	.4429615D-03	.1000000D-08	.2528704D-05	.4216547D-03
93	.6052536D+01	.3000103D-03	.1907559D-02	.1098030D-03	.4430263D-03	.1000000D-08	.2513971D-05	.4198893D-03
94	.6117617D+01	.2985250D-03	.1908950D-02	.1091688D-03	.4430830D-03	.1000000D-08	.2499450D-05	.4181334D-03
95	.6182698D+01	.2970549D-03	.1910301D-02	.1085435D-03	.4431318D-03	.1000000D-08	.2485134D-05	.4163868D-03
96	.6247779D+01	.2955997D-03	.1911614D-02	.1079270D-03	.4431730D-03	.1000000D-08	.2471019D-05	.4146494D-03
97	.6312860D+01	.2941591D-03	.1912888D-02	.1073190D-03	.4432066D-03	.1000000D-08	.2457099D-05	.4129212D-03
98	.6377941D+01	.2927328D-03	.1914125D-02	.1067194D-03	.4432329D-03	.1000000D-08	.2443369D-05	.4112020D-03
99	.6443022D+01	.2912904D-03	.1915338D-02	.1061278D-03	.4432520D-03	.1000000D-08	.2429826D-05	.4094803D-03
100	.6508103D+01	.2898773D-03	.1916513D-02	.1055383D-03	.4432638D-03	.1000000D-08	.2416330D-05	.4077601D-03
101	.6573184D+01	.2884785D-03	.1917652D-02	.1049570D-03	.4432683D-03	.1000000D-08	.2403020D-05	.4060495D-03
102	.6638265D+01	.2870936D-03	.1918755D-02	.1043836D-03	.4432659D-03	.1000000D-08	.2389893D-05	.4043483D-03
103	.6703346D+01	.2857224D-03	.1919822D-02	.1038180D-03	.4432566D-03	.1000000D-08	.2376942D-05	.4026563D-03
104	.6768427D+01	.2843646D-03	.1920854D-02	.1032599D-03	.4432407D-03	.1000000D-08	.2364163D-05	.4009735D-03
105	.6833508D+01	.2830198D-03	.1921852D-02	.1027091D-03	.4432182D-03	.1000000D-08	.2351552D-05	.3992998D-03
106	.6898589D+01	.2816879D-03	.1922817D-02	.1021654D-03	.4431855D-03	.1000000D-08	.2339105D-05	.3976349D-03
107	.6963670D+01	.2803684D-03	.1923750D-02	.1016287D-03	.4431546D-03	.1000000D-08	.2326818D-05	.3959790D-03
108	.7028751D+01	.2790612D-03	.1924651D-02	.1010988D-03	.4431137D-03	.1000000D-08	.2314686D-05	.3943317D-03
109	.7093832D+01	.2777660D-03	.1925520D-02	.1005756D-03	.4430670D-03	.1000000D-08	.2302705D-05	.3926931D-03
110	.7158914D+01	.2764825D-03	.1926359D-02	.1000588D-03	.4430145D-03	.1000000D-08	.2290873D-05	.3910630D-03
111	.7223995D+01	.2752106D-03	.1927168D-02	.9954831D-04	.4429564D-03	.1000000D-08	.2279186D-05	.3894413D-03
112	.7289076D+01	.2739500D-03	.1927948D-02	.9904403D-04	.4428929D-03	.1000000D-08	.2267641D-05	.3878280D-03
113	.7354157D+01	.2727005D-03	.1928699D-02	.9854579D-04	[illegible]	.1000000D-08	.2256233D-05	.3862230D-03
114	.7419238D+01	.2714619D-03	.1929422D-02	.9805345D-04	.4427500D-03	.1000000D-08	.2244961D-05	.3846261D-03
115	.7484319D+01	.2702340D-03	.1930117D-02	.9756689D-04	.4426708D-03	.1000000D-08	.2233821D-05	.3830373D-03
116	.7549400D+01	.2690165D-03	.1930785D-02	.9708598D-04	.4425866D-03	.1000000D-08	.2222811D-05	.3814565D-03
117	.7614481D+01	.2679093D-03	.1931427D-02	.9661060D-04	.4424975D-03	.1000000D-08	.2211927D-05	.3798837D-03
118	.7679562D+01	.2666123D-03	.1932042D-02	.9614062D-04	.4424033D-03	.1000000D-08	.2201166D-05	.3783187D-03
119	.7744643D+01	.2654251D-03	.1932631D-02	.9567594D-04	.4423052D-03	.1000000D-08	.2190527D-05	.3767615D-03
120	.7809724D+01	.2642477D-03	.1933195D-02	.9521645D-04	.4422022D-03	.1000000D-08	.2180007D-05	.3752120D-03
121	.7874805D+01	.2630799D-03	.1933735D-02	.9476203D-04	.4420946D-03	.1000000D-08	.2169603D-05	.3736702D-03
122	.7939886D+01	.2619216D-03	.1934250D-02	.9431258D-04	.4419827D-03	.1000000D-08	.2159313D-05	.3721359D-03
123	.8004967D+01	.2607724D-03	.1934741D-02	.9386802D-04	.4418665D-03	.1000000D-08	.2149134D-05	.3706091D-03
124	.8070048D+01	.2596324D-03	.1935208D-02	.9342823D-04	.4417461D-03	.1000000D-08	.2139065D-05	.3690897D-03
125	.8135129D+01	.2585014D-03	.1935652D-02	.9299312D-04	.4416216D-03	.1000000D-08	.2129104D-05	.3675778D-03
126	.8200210D+01	.2573792D-03	.1936074D-02	.9256262D-04	.4414930D-03	.1000000D-08	.2119287D-05	.3660731D-03

127	.8265291D+01	.2562656D-03	.1936473D-02	.9213661D-04	.4413605D-03	.1000000D-08	.2109494D-05	.3645756D-03
128	.8330372D+01	.2551606D-03	.1936850D-02	.9171503D-04	.4412241D-03	.1000000D-08	.2099841D-05	.3630854D-03
129	.8395453D+01	.2540440D-03	.1937213D-02	.9129778D-04	.4410839D-03	.1000000D-08	.2090288D-05	.3615949D-03
130	.8460534D+01	.2529462D-03	.1937554D-02	.9088092D-04	.4409397D-03	.1000000D-08	.2080744D-05	.3601062D-03
131	.8525615D+01	.2518569D-03	.1937873D-02	.9046850D-04	.4407917D-03	.1000000D-08	.2071301D-05	.3586249D-03
132	.8590696D+01	.2507762D-03	.1938171D-02	.9006038D-04	.4406399D-03	.1000000D-08	.2061957D-05	.3571511D-03
133	.8655777D+01	.24970[illegible]8D-03	.1938447D-02	.8965648D-04	.4404845D-03	.1000000D-08	.2052710D-05	.3556846D-03
134	.8720858D+01	.2486396D-03	.1938702D-02	.8925671D-04	.4403254D-03	.1000000D-08	.2043557D-05	.3542253D-03
135	.8785939D+01	.2475835D-03	.1938936D-02	.8886100D-04	.4401628D-03	.1000000D-08	.2034497D-05	.3527732D-03
136	.8851020D+01	.2465353D-03	.1939150D-02	.8846925D-04	.4399967D-03	.1000000D-08	.2025528D-05	.3513282D-03
137	.8916101D+01	.2454949D-03	.1939344D-02	.8808140D-04	.4398272D-03	.1000000D-08	.2016648D-05	.3498903D-03
138	.8981182D+01	.2444622D-03	.1939518D-02	.8769736D-04	.4396545D-03	.1000000D-08	.2007856D-05	.3484593D-03
139	.9046263D+01	.2434371D-03	.1939673D-02	.8731707D-04	.4394784D-03	.1000000D-08	.1999149D-05	.3470353D-03
140	.9111344D+01	.2424194D-03	.1939809D-02	.8694045D-04	.4392993D-03	.1000000D-08	.1990526D-05	.3456181D-03
141	.9176425D+01	.2414091D-03	.1939927D-02	.8656744D-04	.4391170D-03	.1000000D-08	.1981986D-05	.3442077D-03
142	.9241507D+01	.2404060D-03	.1940026D-02	.8619797D-04	.4389316D-03	.1000000D-08	.1973527D-05	.3428040D-03
143	.9306588D+01	.2394100D-03	.1940107D-02	.8583197D-04	.4387433D-03	.1000000D-08	.1965147D-05	.3414071D-03
144	.9371669D+01	.2384210D-03	.1940170D-02	.8546939D-04	.4385520D-03	.1000000D-08	.1956845D-05	.3400167D-03
145	.9436750D+01	.2374389D-03	.1940215D-02	.8[illegible]11015D-04	.4383579D-03	.1000000D-08	.1948621D-05	.3386329D-03
146	.9501831D+01	.2364636D-03	.1940244D-02	.8475421D-04	.4381610D-03	.1000000D-08	.1940471D-05	.3372556D-03
147	.9566912D+01	.2354951D-03	.1940255D-02	.8440150D-04	.4379613D-03	.1000000D-08	.1932396D-05	.3358868D-03
148	.963[illegible]993D+01	.2345331D-03	.1940250D-02	.8405197D-04	.4377589D-03	.1000000D-08	.1924393D-05	.3345204D-03
149	.9697074D+01	.2335777D-03	.1940229D-02	.8370557D-04	.4375538D-03	.1000000D-08	.1916462D-05	.3331624D-03
150	.9762155D+01	.2326287D-03	.1940191D-02	.8336224D-04	.4373462D-03	.1000000D-08	.1908602D-05	.3318107D-03
151	.9827236D+01	.2316861D-03	.1940137D-02	.8302193D-04	.4371360D-03	.1000000D-08	.1900810D-05	.3304652D-03
152	.9892317D+01	.2307497D-03	.1940068D-02	.8268459D-04	.4369233D-03	.1000000D-08	.1893087D-05	.3291260D-03
153	.9957398D+01	.2298194D-03	.1939983D-02	.8235018D-04	.4367081D-03	.1000000D-08	.1885430D-05	.3277929D-03
154	.1002248D+02	.2288953D-03	.1939883D-02	.8201864D-04	.4364906D-03	.1000000D-08	.1877840D-05	.3264659D-03

Appendix E

WALL-SPRAY MODEL, SAMPLE INPUT AND OUTPUT

```
C***********************************************************************
C
C     WALL-SPRAY MODEL
C
C     M. F. ALBERT
C
C     THE WALL-SPRAY MODEL SIMULATES THE REMOVAL OF GASEOUS MOLECULAR
C     IODINE, I2, BY WATER SPRAYS AND ALSO BY THE WATER ON THE WALLS
C     OF THE CONTAINMENT VESSEL.  THIS MODEL IS ESSENTIALLY THE SPRAY
C     MODEL WITH THE ADDITION OF A SIMULATION OF THE ABSORPTION OF A
C     GAS BY A FALLING LIQUID FILM.  A TWO-RESISTANCE MODEL IS USED TO
C     DESCRIBE THE MASS TRANSFER.  A RUNGE-KUTTA-FELHBURG 5(4) NUMERICAL
C     INTEGRATION ROUTINE IS USED TO INTEGRATE THE IODINE HYDROLYSIS
C     REACTIONS.  SUBROUTINE CALLED FROM THIS MAIN PROGRAM ARE ITTER,
C     FUNCTN, WALL AND POOL.  THIS PROGRAM IS DESIGNED TO RUN ON A
C     PDP-10 COMPUTER BUT SHOULD BE EASILY CONVERTED TO RUN ON ANY
C     FORTRAN COMPUTER.
C
C***********************************************************************
C
      IMPLICIT DOUBLE PRECISION (A-H,K-Z)
      IMPLICIT INTEGER (I-J)
C
      DIMENSION W(8),WOLD(8),K1(7),K2(7),K3(7),R(7),WB(7),
     1     DELTA(7),WES(7),F(7),K4(7),K5(7),K6(7),TOL(7),
     2     CCB(7),CC(7),CONPOL(8),CONWAL(8,300)
C
      READ (58,*)A,HMIN,HMAX,IN
      READ (49,*)TOLER
      READ (31,*)TEMPG,TEMPL,PRESS,DIAM,SAD,CI2SP,CISP
      READ (31,*)CHOISP,COISP
      READ (43,*)CI2G,CHSP,FLRAT,DURTM
      READ (31,*)CIO3SP,CI3SP
      READ (30,*)CDIAM,HEIGHT,WFRAC,WHT
C
9     FORMAT('  CONCENTRATION OF THE DROPS',/)
10    FORMAT('AT A TEMPERTURE OF THE GAS ',F6.2,' DEGRESS KELVIN'/
     1 'THE VISCOSITY OF THE LIQUID (CP)=',E15.7/
     2 'THE VISCOSITY OF THE GAS (CP) =',E15.7/
     3 'THE PARTITION COEFFICIENT IS =',E15.7/
     4 'THE DENSITY OF THE LIQUID (GMS/CC) =',E15.7/
     5 'THE DENSITY OF THE GAS (GMS/CC) =',E15.7)
11    FORMAT('THE DIFFUSION COEFFICIENT FOR THE GAS (SQ CM/SEC)=',E15.7
     1 /'THE DIFFUSION COEFFICIENT FOR THE LIQUID (SQ CM/SEC)=',E15.7/
     2 'THE GAS-SIDE MASS TRANSFER COEFFICIENT (CM/SEC)='E15.7/
     3 'THE LIQUID-SIDE MASS TRANSFER COEFFICIENT (CM/SEC)=',E15.7/
     4'THE OVERALL LIQUID-SIDE MASS TRANSFER COEFFICIENT (CM/SEC)=',E15.
     57,/, 'THE VOLUME FOR ONE DROP (LITERS)=',E15.7/
     6 'THE SURFACE AREA FOR ONE DROP (SQ CM)=',E15.7/
     7 'THE EXPOSURE TIME FOR THE DROP IS (SEC)=',E15.7/
     8 'THE REYNOLDS NUMBER FOR THE DROP =',E15.7/
     9 'THE TERMINAL VELOCITY OF THE DROP (CM/SEC) =',E15.7)
12    FORMAT(I5)
13    FORMAT('                      I2 = ',E15.7/
     2'                      I- = ',E15.7/
     3'                     HOI = ',E15.7/
     4'                    IO3- = ',E15.7/
     5'                      H+ = ',E15.7/
     6'                     IO- = ',E15.7/
     7'                     I3- = ',E15.7/)
```

```
14     FORMAT('THE FINAL CONCENTRATION OF THE LIQUID IS (MOLES/LITER) :')
15     FORMAT('THE NUMBER OF MOLES OF IODINE (I2) REMOVED IS =',E15.7,/
      1        'THE NUMBER OF GRAMS OF IODINE REMOVES IS =',E15.7,/)
16     FORMAT('THE FINAL CONCENTRATION OF IODINE (I2) IN THE GAS IS ',
      1E15.7,' (MOLES/LITER)',/)
17     FORMAT('       TIME              MOLES RMD          CON GAS         SUM MLS RM
      1D',/)
18     FORMAT('    CONCENTRATION OF THE SPRAYED SOLUTION IN THE SUMP ',/)
19     FORMAT('     N     TIME              I2               I-             HOI
      1     IO3-          H+           IO-           I3-',/)
21     FORMAT('STEP SIZE BELOW STEP MIN',D15.7)
22     FORMAT(I5,8D13.7)
23     FORMAT(4D15.7)
32     FORMAT('THE NUMBER OF DROPS IN THE CONTAINMENT IS',E15.7/
      1 'THE DROP FLUX (NUMBER OF DROPS/SQ CM MIN) =',E15.7/
      2 'THE CONTAINMENT VOLUME (LITERS) =',E15.7/
      3 'THE NUMBER OF OUTER LOOPS =',I6/)
33     FORMAT(/' THE NUMBER OF GRAMS OF IODINE REMOVED IN THE EXPERIMENT
      1IS ',E15.7,/,'RESULTING IN AN ERROR OF ',E15.7,' PERCENT.'/)
34     FORMAT(//'THE INITIAL CONCENTRATION IN THE GAS OF',E15.7,
      1' (MOLES/LITER)',/,
      2'THE DURATION OF THE SPRAY (MIN) ',E15.7,/,
      3'THE VOLUME OF LIQUID SPRAYED (LITERS) ',E15.7,/,
      4'AND A SPRAY FLOW RATE OF ',E15.7,' (LITERS/MIN)',/,
      5'THE INITIAL CONCENTRATION OF THE LIQUID (MOLES/LITER) :')
C
       WRITE(50,9)
       WRITE(50,19)
       WRITE(52,18)
       WRITE(52,19)
       WRITE(51,17)
C
5       SFA=3.1416D00*SAD**2
       VOLD=(3.1416D00*DIAM**3.D00)/(6.D00*1.0D3)
       CI2GI=CI2G
C
       TEMPG4=TEMPG**4
       TEMPG3=TEMPG**3
       TEMPG2=TEMPG**2
C
       TEMPL4=TEMPL**4
       TEMPL3=TEMPL**3
       TEMPL2=TEMPL**2
C
       VSL1=1.8662866D-8*TEMPL4-2.6333695D-5*TEMPL3+1.3970607D-2*TEMPL2
       VSL2=-3.3074806D00*TEMPL+2.9558666D2
       VISLIQ=VSL1+VSL2
C
       PC1=9.981476D-7*TEMPL4-1.5730121D-3*TEMPL3+9.2785676D-1*TEMPL2
       PC2=-2.4288388D2*TEMPL+2.3824847D4
       PC=PC1+PC2
C
       DNL1=6.0251147D-9*TEMPL3-9.1329604D-6*TEMPL2
       DNL2=3.573572D-3*TEMPL+5.8358882D-1
       DENLIQ=DNL1+DNL2
C
       VSA1=-2.8713293D-15*TEMPG4+1.6909463D-11*TEMPG3-4.015468D-8*TEMPG2
       VSA2=6.5679429D-5*TEMPG+1.9523691D-3
       VISGAS=VSA1+VSA2
C
       TMP=5.178D-3*TEMPG
       OMEGA1=TMP**3*(-6.19047619D-2)+4.657142857D-1*TMP**2
       OMEGA2=TMP*(-1.304238095D00)+2.315428571D00
       OMEGA=OMEGA1+OMEGA2
C
       MLWT=1/2.9D1+1/2.53809D2
```

```
      DIFGAS=1.858D-3*TEMPG**1.5*MLWT**0.5/(PRESS*4.4355D00**2*OMEGA)
      DIFLIQ=3.91D-8*TEMPL/VISLIQ
C
      DNG1=8.2892055D-16*TEMPG4-4.2656962D-12*TEMPG3+8.0228283D-9*TEMPG2
      DNG2=-6.8325529D-6*TEMPG+2.6129391D-3
      DENGLS=DNG1+DNG2
C
      GSM1=0.83D00*((DENLIQ-DENGAS)/DENGAS)**0.25*9.81D2**0.25
      GSM2=(VISGAS/(1.0D2*DENGAS))**-0.17*DIFGAS**0.67*DIAM**-0.25
      KGI2=GSM1*GSM2
C
      ND1=4.D00*DENGAS*(DENLIQ-DENGAS)*9.81D2*DIAM**3
      ND2=3.0D00*(VISGAS/1.0D2)**2
      ND=ND1/ND2
C
      WW=DLOG10(ND)
C
      NRE1=(-1.81391D00+1.34671D00*WW-0.12427D00*WW**2+6.344D-3*WW**3)
      NRE=1.0D1**NRE1
C
      TRMVEL=NRE*(VISGAS/1.0D2)/(DIAM*DENGAS)
C
      EXPTM=HEIGHT*1.0D2/TRMVEL
C
      KLI2O=(4.0D00*DIFLIQ*TRMVEL/(3.1415D00*DIAM))**0.5
C
      KLOV=KGI2*KLI2O/(PC*KLI2O+KGI2)
C
      CCSA=(CDIAM/2.0D00)**2.0*3.14149265D00
C
      DPMIN=FLRAT/VOLD
C
      FLXDP=DPMIN/(CCSA*1.0D4)
C
      ADARA=6.0D1/(EXPTM*FLXDP)
C
      ILOOP=DURTM*6.0D1/EXPTM+1.0D00
C
      VOLCON=ADARA*HEIGHT/1.0D1
C
      VOLSP=FLRAT*DURTM
C
      NUMDPS=DPMIN*EXPTM/6.0D1
C
      CVOL=CCSA*HEIGHT*1.0D3
C
      WLTM=(HEIGHT-WHT)*1.0D2/TRMVEL
C
      WMFR=(WFRAC*FLRAT*DENLIQ*1.6667D1/(CDIAM*3.141593))
C
      WFILM=(3.0D00*VISLIQ*WMFR*1.0D-4/(DENLIQ**2*9.81D2))**0.33
C
      WVEL=WMFR/(DENLIQ*WFILM*1.0D2)
C
      WVOL=FLRAT*WFRAC*EXPTM/6.0D1
C
      IM=0
      IMAX=WHT*1.0D2/(EXPTM*WVEL)+1.0D00
C
      KLW=(6.0D00*DIFLIQ*WMFR/(1.0D2*3.141593*DENLIQ*WFILM*EXPTM*WVEL))
      KLW=KLW**0.5
C
      WAREA=WVOL/WFILM
C
      WRITE(23,12) ILOOP
      WRITE (22,10) TEMPG,VISLIQ,VISGAS,PC,DENLIQ,DENGAS
      WRITE (22,11) DIFGAS,DIFLIQ,KGI2,KLI2O,KLOV,VOLD,SFA,EXPTM,NRE,
```

```
     1                  TEMVEL
      WRITE (22,32)NUMDPS,FLIDP,CVOL,ILOOP
      WRITE (22,34)CI2G,DURTM,VOLSP,FLRAT
C
C     DETERMINE THE EQUILIBRIUM CONSTANTS FOR EQUATIONS 4, 5 AND 6
C     (EQUATIONS 23, 24 AND 25)
C
      RK6=-4.098D00-3245.2D00/TEMPL+2.2363D5/(TEMPL**2)-3.984D7/(TEMPL**
     13)+(13.957D00-1262.3D00/TEMPL+8.5641D5/(TEMPL**2))*DLOG(DENLIQ)
      RK6=10**(RK6)
C
      RK5=10**(2800.48D00+0.7335D00*TEMPL-80670.0D00/TEMPL
     1-1115.1D00*DLOG10(TEMPL))
C
      RK4=DEXP(3727.86D00/TEMPL-11.6326D00+0.0192212D00*TEMPL)
C
      TOUTPL=EXPTM/2.0D1
      SPA1=SPA*NUMDPS
      VOLD1=NUMDPS*VOLD
      TOLD=A
      Q=1.0D-1
      IF (WOLD(5) .GT. 0.0D00)GOTO 38
      WOLD(8)=0.0D00
      GOTO 37
38    WOLD(8)=RK6/WOLD(5)
C
37    WRITE (22,13)CI2SP,CISP,CHOISP,CIO3SP,CHSP,COISP,
     1               CI3SP
      WRITE(50,22)I,TIME,CI2SP,CISP,CHOISP,CIO3SP,CHSP,COISP
     1               ,CI3SP
C
      DO 1100 II=1,ILOOP
      IMK=IMK+1.0D00
      H=1.0D-2
      TOLD=A
      B=EXPTM
C
C     INITIALIZE THE DROP CONCENTRATION
C
      CI2L=CI2SP
      WOLD(2)=CISP
      WOLD(5)=CHSP
      WOLD(4)=CIO3SP
      WOLD(7)=CI3SP
      WOLD(3)=CHOISP
      WOLD(6)=COISP
C
      SUMMOL=0.0D00
      WALMOL=0.0D00
      IFLAG=1
      SPA=SPA1
      VOLD=VOLD1
C
C     BEGIN THE RUNGE-KUTTA-FELHBURG ROUTINE TO DETERMINE THE
C     ABSORPTION BY THE SPRAY DROPLETS
C
1     T=TOLD
C
C     DETERMINE THE MASS TRANSFER TO THE SPRAY DROPLETS
C
      WOLD(1)=CI2L
      NMOL=WOLD(1)*VOLD
      MOLTR=KLOV*H*SPA*(CI2G*PC-WOLD(1))/1.0D3
      WOLD(1)=(NMOL+MOLTR)/VOLD
C
C     CALCULATE K'S
```

```
C
      DO 30 J=1,IN
       W(J)=WOLD(J)
30    CONTINUE
C
      CALL FUNCTN(W,WOLD,F,IN)
C
      DO 40 J=1,IN
       K1(J)=H*F(J)
40    CONTINUE
C
      DO 50 J=1,IN
       W(J)=WOLD(J)+K1(J)/4.0D00
50    CONTINUE
C
      CALL FUNCTN(W,WOLD,F,IN)
C
      DO 60 J=1,IN
       K2(J)=H*F(J)
60    CONTINUE
C
      DO 80 J=1,IN
       W(J)=WOLD(J)+3.0D00*K1(J)/3.2D1+9.0D00*K2(J)/3.2D1
80    CONTINUE
C
      CALL FUNCTN(W,WOLD,F,IN)
C
      DO 90 J=1,IN
       K3(J)=H*F(J)
90    CONTINUE
C
      DO 110 J=1,IN
       W(J)=WOLD(J)+1.932D3*K1(J)/2.197D3-7.2D3*K2(J)/2.197D3
     1      +7.296D3*K3(J)/2.197D3
110   CONTINUE
C
      CALL FUNCTN(W,WOLD,F,IN)
C
      DO 120 J=1,IN
       K4(J)=H*F(J)
120   CONTINUE
C
      DO 130 J=1,IN
       W(J)=WOLD(J)+4.39D2*K1(J)/2.16D2-8.0D00*K2(J)+3.68D3*K3(J)/5.13D2
     1      -8.45D2*K4(J)/4.104D3
130   CONTINUE
C
      CALL FUNCTN(W,WOLD,F,IN)
C
      DO 140 J=1,IN
       K5(J)=H*F(J)
140   CONTINUE
C
      DO 150 J=1,IN
       W(J)=WOLD(J)-8.D00*K1(J)/2.7D1+2.D00*K2(J)-3.544D3*K3(J)/2.565D3
     1      +1.859D3*K4(J)/4.104D3-1.1D1*K5(J)/4.0D1
150   CONTINUE
C
      CALL FUNCTN(W,WOLD,F,IN)
C
      DO 160 J=1,IN
       K6(J)=H*F(J)
160   CONTINUE
C
C
C     DETERMINE THE NEW CONCENTRATION IN THE SPRAY DROPLETS FOR ALL OF
```

```
C     THE IODINE HYDROLYSIS SPECIES AND CHECK ERROR
C
      DO 100 J=1,IN
       WB(J)=WOLD(J)+1.6D1*K1(J)/1.35D2+6.656D3*K3(J)/1.2825D4+
     1       2.8561D4*K4(J)/5.643D4-9.0D00*K5(J)/5.0D1+2.0D00*K6(J)/5.5D1
       R(J)=ABS(K1(J)/3.6D2-1.28D2*K3(J)/4.275D3-2.197D3*K4(J)/7.524D4
     1          +K5(J)/5.0D1+2.0D00*K6(J)/5.5D1)/H
       TOL(J)=ABS(WB(J)*TOLER)
       DELTA(J)=0.84*(TOL(J)/R(J))**0.25
100   CONTINUE
C
      DO 500 J=1,IN
       IF(R(J) .GT. TOL(J))GOTO 900
500   CONTINUE
C
      DO 510 J=1,IN
       WOLD(J)=WB(J)
510   CONTINUE
C
C     DETERMINE THE EQUILIBRIUM CONCENTRATIONS OF EQUATIONS 23, 24 AND
C     25
C
      BB=-1.0D00-(WOLD(2)+WOLD(1))*RK4
      C=WOLD(2)*WOLD(1)*RK4-WOLD(7)
      D=-BB/(2.0D00*RK4)
      E=((BB**2.0D00-4.0D00*RK4*C)**0.5D00)/(2.0D00*RK4)
      V=D-E
C
      IF(V .LT. 1.0D-18 .AND. V .NE. 0.0D00) CALL ITTER(WOLD,RK4,C,V)
C
      WOLD(7)=WOLD(7)+V
      WOLD(1)=WOLD(1)-V
      WOLD(2)=WOLD(2)-V
C
      IF(IN .EQ. 4)GOTO 600
C
      RR=WOLD(6)+WOLD(5)+RK5
      S=-RK5*WOLD(3)+WOLD(6)*WOLD(5)
      M=(-RR+(RR*RR-4.0D00*S)**0.5)/2.0D00
      WOLD(5)=WOLD(5)+M
C
      GOTO 605
C
600   M=(RK5*WOLD(3)-WOLD(6)*WOLD(5))/(WOLD(5)+RK5)
C
605   WOLD(6)=WOLD(6)+M
      WOLD(3)=WOLD(3)-M
C
      IF(IN .EQ. 4)GOTO 614
C
      U=WOLD(8)*WOLD(5)-RK6
      VV=WOLD(8)+WOLD(5)
      X=(-VV+(VV*VV-4.0D00*U)**0.5)/2.0D00
      WOLD(5)=WOLD(5)+X
      WOLD(8)=WOLD(8)+X
C
614   IF(IFLAG .EQ. 2 .OR. TOLD .LT. WLTM)GOTO 615
      IFLAG=2
C
      DO 620 J=1,7
       CONWAL(J,1)=WOLD(J)
620   CONTINUE
C
      SPA=SPA1*(1-WFRAC)
      VOLD=VOLD1*(1.0D00-WFRAC)
C
```

```
615   TOLD=TOLD+H
      SUMMOL=SUMMOL+MOLTR
      FHT=TRMVEL*TIME
      CI2L=WB(1)
      FHT=TOLD*TRMVEL
      DEL=DELTA(1)
C
      IF(IN .EQ. 1)GOTO 905
C
      DO 520 J=2,IN
       IF(DEL .LT. DELTA(J))GOTO 520
       DEL=DELTA(J)
520   CONTINUE
C
      GOTO 905
C
C     DETERMINE NEW STEP SIZE
C
900   DEL=DELTA(J)
C
905   IF(DEL .GT. Q) GOTO 910
      HNEW=Q*H
      GOTO 1000
C
910   IF(DEL .LT. 4.0)GOTO 920
      HNEW=4.0D00*H
      GOTO 1000
C
920   HNEW=DEL*H
C
C     CHECK NEW STEP SIZE WITH MAX AND MIN STEP SIZE
C
1000  IF (HNEW .LT. HMAX)GOTO 930
      HNEW=HMAX
C
930   IF (HNEW .LT. HMIN)GOTO 1111
      LEFT=B-TOLD-HNEW
C
      IF(LEFT .GT. 0.0)GOTO 5000
      HNEW=B-TOLD
C
5000  H=HNEW
C
      IF(TOLD .GE. B)GOTO 999
C
      GOTO 1
C
C
C     BEGIN DETERMINATION OF THE REMOVAL BY THE WALLS
C
999   TIME=TIME+TOLD/6.0D1
C
      FHT=TIME*TRMVEL
C
C      WRITE(5,43)II,ILOOP,IM,IMAX
43    FORMAT(4I6)
      IF(IM .GE. IMAX)GOTO 79
      IM=IM+1
C
C     DETERMINE THE MASS TRANSFER TO THE WATER ON THE WALLS
C
79    DO 84 IQ=IM,1,-1
C      WRITE(5,44)IQ,IM
44    FORMAT(2I6)
       WSUM=0.0D00
       CALL WALL(CONWAL,A,B,HMIN,HMAX,IN,DIFLIQ,WMFR,WSUM,DENLIQ,KLW,
```

```
     1WAREA,WVOL,TOLER,WFILM,WVEL,FLBAT,WFRAC,IQ,RK4,RK5,RK6,CI2G,PC,
     2EXPTM)
C
      WALMOL=WALMOL+WSUM
C
      DO 85 J=1,7
       CONWAL(J,IQ+1)=CONWAL(J,IQ)
85    CONTINUE
C
84    CONTINUE
C
C     DETERMINE THE CONCENTRATION IN THE SUMP
C
      CALL POOL(CONPOL,A,B,HMIN,HMAX,IN,TOLER)
C
      IF(IM .GT. IMAX)GOTO 83
C
      DO 81 J=1,7
       CONPOL(J)=(CONPOL(J)*POLVOL+WOLD(J)*VOLD)/(POLVOL+VOLD)
81    CONTINUE
C
      POLVOL=POLVOL+VOLD
      GOTO 87
C
83    DO 82 J=1,7
       CONPOL(J)=(CONPOL(J)*POLVOL+CONWAL(J,IMAX+1)*WVOL+WOLD(J)*VOLD)/(
     1WVOL+VOLD+POLVOL)
82    CONTINUE
C
      POLVOL=POLVOL+VOLD+WVOL
87    CI2G=(CI2G*CVOL-(SUMMOL+WALMOL))/CVOL
C
      SUM=SUMMOL+SUM+WALMOL
C
      WRITE(50,22)II,TIME,WOLD(1),WOLD(2),WOLD(3),WOLD(4),WOLD(5),
     1           WOLD(6),WOLD(7)
      WRITE(52,22)II,TIME,CONPOL(1),CONPOL(2),CONPOL(3),CONPOL(4),
     1           CONPOL(5),CONPOL(6),CONPOL(7)
      WRITE(51,23)TIME,SUMMOL,CI2G,SUM
C
1100  CONTINUE
C
C     DETERMINE THE TRANSFER BY THE WATER STILL DRAINING OFF THE WALLS
C
91    DO 95 IQ=1,IM
       CALL WALL(CONWAL,A,B,HMIN,HMAX,IN,DIFLIQ,WMFR,WSUM,DENLIQ,KLW,
     1WAREA,WVOL,TOLER,WFILM,WVEL,FLBAT,WFRAC,IQ,RK4,RK5,RK6,CI2G,PC,
     2EXPTM)
C
      WALMOL=WALMOL+WSUM
      SUM=SUM+WSUM
      CI2G=(CI2G*CVOL-WSUM*GASFAC)/CVOL
C
      CALL POOL(CONPOL,A,B,HMIN,HMAX,IN,TOLER)
C
      DO 92 J=1,7
       CONPOL(J)=(CONPOL(J)*POLVOL+CONWAL(J,IQ)*WVOL)/(WVOL+POLVOL)
92    CONTINUE
C
      POLVOL=POLVOL+WVOL
95    CONTINUE
C
      IF(IM .LE. 1 )GOTO 2000
      IM=IM-1
      GOTO 91
```

```
      WRITE(50,22) II,TIME,WOLD(1),WOLD(2),WOLD(3),WOLD(4),WOLD(5),
     1             WOLD(6),WOLD(7)
      WRITE(52,22) II,TIME,CONPOL(1),CONPOL(2),CONPOL(3),CONPOL(4),
     1             CONPOL(5),CONPOL(6),CONPOL(7)
C
2000  SUMGRM=2.53809D2*SUM
C
      WRITE(22,16) CI2G
      WRITE(22,15) SUM,SUMGRM
      WRITE(22,14)
      WRITE(22,13) CONPOL(1),CONPOL(2),CONPOL(3),CONPOL(4),CONPOL(5),
     1             CONPOL(6),CONPOL(7)
      GOTO 3000
C
1111  WRITE(40,21) HNEW
C
3000  STOP
      END
```

```
C*****************************************************************************
C
C     SUBROUTINE WALL
C
C     THIS SUBROUTINE IS CALLED FROM THE ROUTINE WALL-SPRAY.  THIS
C     SUBROUTINE DETERMINES THE REMOVAL OF MOLECULAR IODINE BY THE
C     WATER FLOWING DOWN THE WALLS OF A CONTAINMENT VESSEL.  THE
C     ALGORITHM USED FOR THE MASS TRANSFER IS FOR A FALLING LIQUID
C     FILM AND A RUNGE-KUTTA-FELHBURG 5(4) ROUTINE IS USED TO
C     NUMERICALLY INTEGRATE THE IODINE HYDROLYSIS REACTIONS.
C
C*****************************************************************************
C
      SUBROUTINE WALL(CONWAL,A,B,HMIN,HMAX,IN,DIFLIQ,WMFR,WSUM,DENLIQ,
     1KLW,WAREA,WVOL,TOLER,WFILM,WVEL,FLRAT,WFRAC,IQ,RK4,RK5,RK6,CI2G,PC
     2,EXPTM)
C
      IMPLICIT DOUBLE PRECISION (A-H,K-Z)
      IMPLICIT INTEGER (I-J)
C
      DIMENSION W(8),CONWAL(8,300),K1(7),K2(7),K3(7),R(7),WB(7),
     1     DELTA(7),WES(7),F(7),K4(7),K5(7),K6(7),TOL(7),WALCON(2)
C
21    FORMAT('STEP SIZE BELOW STEP MIN',D15.7)
C
      CI2W=CONWAL(1,IQ)
      TOLD=A
      Q=1.0D-1
      H=1.0D-2
C
      CONWAL(8,IQ)=RK6/CONWAL(5,IQ)
C
C     USE SECANT METHOD TO DETERMINE THE LOG MEAN BULK CONCENTRATION
C     IN THE LIQUID
C
1     CONWAL(1,IQ)=CI2W
      WNMOL=CONWAL(1,IQ)*WVOL/1.0D3
      P0=CONWAL(1,IQ)*1.02D00
      P1=CONWAL(1,IQ)*1.05D00
      Q0=H*KLW/WFILM*(P0-CONWAL(1,IQ))/DLOG((CI2G*PC-CONWAL(1,IQ))/(CI2G
     1*PC-P0))+CONWAL(1,IQ)-P0
55    Q1=H*KLW/WFILM*(P1-CONWAL(1,IQ))/DLOG((CI2G*PC-CONWAL(1,IQ))/(CI2G
     1*PC-P1))+CONWAL(1,IQ)-P1
      CI2LM=(Q1*P0-Q0*P1)/(Q1-Q0)
      CHECK=ABS(CI2LM-P1)/P1
      IF(CHECK .LT. 1.0D-3)GOTO 59
      P0=P1
      Q0=Q1
      P1=CI2LM
      GOTO 55
C
59    WMOLTR=WFILM*(CI2LM-CONWAL(1,IQ))*WAREA*H/(1.0D3*EXPTM)
      WSUM=WMOLTR+WSUM
      CONWAL(1,IQ)=CONWAL(1,IQ)+WMOLTR*1.0D3/WVOL
C
C     BEGIN RUNGE-KUTTA-FELHBURG ROUTINE
C
C     CALCULATE K'S
C
      DO 30 J=1,IN
       W(J)=CONWAL(J,IQ)
30    CONTINUE
C
```

```
      CALL FUNCTN(W,CONWAL,F,IN)
C
      DO 40 J=1,IN
       K1(J)=H*F(J)
40    CONTINUE
C
      DO 50 J=1,IN
       W(J)=CONWAL(J,IQ)+K1(J)/4.0D00
50    CONTINUE
C
      CALL FUNCTN(W,CONWAL,F,IN)
C
      DO 60 J=1,IN
       K2(J)=H*F(J)
60    CONTINUE
C
      DO 80 J=1,IN
       W(J)=CONWAL(J,IQ)+3.0D00*K1(J)/3.2D1+9.0D00*K2(J)/3.2D1
80    CONTINUE
C
      CALL FUNCTN(W,CONWAL,F,IN)
C
      DO 90 J=1,IN
       K3(J)=H*F(J)
90    CONTINUE
C
      DO 110 J=1,IN
       W(J)=CONWAL(J,IQ)+1.932D3*K1(J)/2.197D3-7.2D3*K2(J)/2.197D3
     1      +7.296D3*K3(J)/2.197D3
110   CONTINUE
C
      CALL FUNCTN(W,CONWAL,F,IN)
C
      DO 120 J=1,IN
       K4(J)=H*F(J)
120   CONTINUE
C
      DO 130 J=1,IN
       W(J)=CONWAL(J,IQ)+4.39D2*K1(J)/2.16D2-8.D00*K2(J)+3.68D3*K3(J)/5.
     11 D2-8.45D2*K4(J)/4.104D3
130   CONTINUE
C
      CALL FUNCTN(W,CONWAL,F,IN)
C
      DO 140 J=1,IN
       K5(J)=H*F(J)
140   CONTINUE
C
      DO 150 J=1,IN
       W(J)=CONWAL(J,IQ)-8.D00*K1(J)/2.7D1+2.D00*K2(J)-3.544D3*K3(J)/2.
     1565D3+1.859D3*K4(J)/4.104D3-1.1D1*K5(J)/4.0D1
150   CONTINUE
C
      CALL FUNCTN(W,CONWAL,F,IN)
C
      DO 160 J=1,IN
       K6(J)=H*F(J)
160   CONTINUE
C
C
C     DETERMINE THE NEW CONCENTRATION OF THE IODINE HYDROLYSIS SPECIES
C     IN THE LIQUID ON THE WALLS AND CHECK ERROR
C
      DO 100 J=1,IN
       WB(J)=CONWAL(J,IQ)+1.6D1*K1(J)/1.35D2+6.656D3*K3(J)/1.2825D4+
     1      2.8561D4*K4(J)/5.643D4-9.0D00*K5(J)/5.0D1+2.0D00*K6(J)/5.5D1
```

```
      R(J)=ABS(K1(J)/3.6D2-1.28D2*K3(J)/4.275D3-2.197D3*K4(J)/7.524D4
     1          +K5(J)/5.0D1+2.0D00*K6(J)/5.5D1)/H
      TOL(J)=ABS(WB(J)*TOLER)
      DELTA(J)=0.84*(TOL(J)/R(J))**0.25
100   CONTINUE
C
      DO 500 J=1,IN
       IF(R(J) .GT. TOL(J))GOTO 900
500   CONTINUE
C
      DO 510 J=1,IN
       CONWAL(J,IQ)=WB(J)
510   CONTINUE
C
C     DETERMINE THE EQUILIBRIUM CONCENTRATION OF EQUATION 23, 24 AND
C     25 FOR THE CYLINDRICAL PIECE OF THE WALL
C
      BB=-1.0D00-(CONWAL(2,IQ)+CONWAL(1,IQ))*RK4
      C=CONWAL(2,IQ)*CONWAL(1,IQ)*RK4-CONWAL(7,IQ)
      D=-BB/(2.0D00*RK4)
      E=((BB**2.0D00-4.0D00*RK4*C)**0.5D00)/(2.0D00*RK4)
      V=D-E
C
      IF(V .GT. 1.0D-18 .AND. V .EQ. 0.0D00)GOTO 575
      WALCON(1)=CONWAL(1,IQ)
      WALCON(2)=CONWAL(1,IQ)
      CALL ITTER(WALCON,RK4,C,V)
C
575   CONWAL(7,IQ)=CONWAL(7,IQ)+V
      CONWAL(1,IQ)=CONWAL(1,IQ)-V
      CONWAL(2,IQ)=CONWAL(2,IQ)-V
C
      IF(IN .EQ. 4)GOTO 600
C
      RR=CONWAL(6,IQ)+CONWAL(5,IQ)+RK5
      S=-RK5*CONWAL(3,IQ)+CONWAL(6,IQ)*CONWAL(5,IQ)
      M=(-RR+(R *RR-4.0D00*S)**0.5)/2.0D00
      CONWAL(5,IQ)=CONWAL(5,IQ)+M
      GOTO 605
C
600   M=(RK5*CONWAL(3,IQ)-CONWAL(6,IQ)*CONWAL(5,IQ))/(CONWAL(5,IQ)+RK5)
C
605   CONWAL(6,IQ)=CONWAL(6,IQ)+M
      CONWAL(3,IQ)=CONWAL(3,IQ)-M
C
      IF(IN .EQ. 4)GOTO 615
C
      U=CONWAL(8,IQ)*CONWAL(5,IQ)-RK6
      VV=CONWAL(8,IQ)+CONWAL(5,IQ)
      X=(-VV+(VV*VV-4.0D00*U)**0.5)/2.0D00
      CONWAL(5,IQ)=CONWAL(5,IQ)+X
      CONWAL(8,IQ)=CONWAL(8,IQ)+X
C
615   I=I+1
      TOLD=TOLD+H
C
      CI2W=CONWAL(1,IQ)
      DEL=DELTA(1)
C
      IF(IN .EQ. 1)GOTO 905
C
      DO 520 J=2,IN
       IF(DEL .LT. DELTA(J))GOTO 520
       DEL=DELTA(J)
520   CONTINUE
C
```

```
      GOTO 905
C
C     DETERMINE NEW STEP SIZE
C
900   DEL=DELTA(J)
C
905   IF(DEL .GT. Q)GOTO 910
       HNEW=Q*H
      GOTO 1000
C
910   IF(DEL .LT. 4.0)GOTO 920
       HNEW=4.0D00*H
      GOTO 1000
C
920   HNEW=DEL*H
C
C     CHECK NEW STEP SIZE WITH MAX AND MIN STEP SIZE
C
1000  IF (HNEW .LT. HMAX)GOTO 930
       HNEW=HMAX
C
930   IF (HNEW .LT. HMIN)GOTO 1111
       LEFT=B-TOLD-HNEW
C
      IF(LEFT .GT. 0.0)GOTO 5000
      HNEW=B-TOLD
C
5000  H=HNEW
C
      IF(TOLD .GE. B)GOTO 999
      GOTO 1
C
C
1111  WRITE(40,21)HNEW
999   RETURN
      END
```

```
C*****************************************************************************
C
C       SUBROUTINE POOL
C
C       THIS SUBROUTINE DETERMINES THE CONCENTRATION OF THE IODINE
C       HYDROLYSIS SPECIES IN THE SUMP POOL.  A RUNGE-KUTTA-FELHBURG
C       5(4) ROUTINE IS USED TO INTEGRATE THE IODINE HYDROLYSIS
C       REACTIONS.  THIS SUBROUTINE IS CALL FROM THE WALL-SPRAY
C       ROUTINE.
C
C*****************************************************************************
C
        SUBROUTINE POOL(CONPOL,A,B,HMIN.HMAX,IN,TOLER)
C
        IMPLICIT DOUBLE PRECISION (A-H,K-Z)
        IMPLICIT INTEGER(I-J)
C
        DIMENSION CONPOL(8),CC(7),K1(7),K2(7),K3(7),K4(7),K7(7),K6(7),
     1            TOL(7),DELTA(7),R(7),CCB(7),F(7)
C
21      FORMAT(' STEP SIZE BELOW HMIN ',E15.7)
C
        H=1.0D-2
        Q=1.0D-1
        PTOLD=A
C
C       BEGIN THE RUNGE-KUTTA-FELHBURG ROUTINE
C
C       CALCULATE K'S
C
2       DO 31 J=1,IN
         CC(J)=CONPOL(J)
31      CONTINUE
C
        CALL FUNCTN(CC,CONPOL,F,IN)
C
        DO 41 J=1,IN
         K1(J)=H*F(J)
41      CONTINUE
C
        DO 51 J=1,IN
         CC(J)=CONPOL(J)+K1(J)/4.0D00
51      CONTINUE
C
        CALL FUNCTN(CC,CONPOL,F,IN)
C
        DO 61 J=1,IN
         K2(J)=H*F(J)
61      CONTINUE
C
        DO 81 J=1,IN
         CC(J)=CONPOL(J)+3.0D00*K1(J)/3.2D1+9.0D00*K2(J)/3.2D1
81      CONTINUE
C
        CALL FUNCTN(CC,CONPOL,F,IN)
C
        DO 91 J=1,IN
         K3(J)=H*F(J)
91      CONTINUE
C
        DO 111 J=1,IN
         CC(J)=CONPOL(J)+1.932D3*K1(J)/2.197D3-7.2D3*K2(J)/2.197D3
     1       +7.296D3*K3(J)/2.197D3
```

```
111   CONTINUE
C
      CALL FUNCTN(CC,CONPOL,F,IN)
C
      DO 121 J=1,IN
       K4(J)=H*F(J)
121   CONTINUE
C
      DO 131 J=1,IN
       CC(J)=CONPOL(J)+4.39D2*K1(J)/2.16D2-8.0D00*K2(J)+
     1      3.68D3*K3(J)/5.13D2-8.45D2*K4(J)/4.104D3
131   CONTINUE
C
      CALL FUNCTN(CC,CONPOL,F,IN)
C
      DO 141 J=1,IN
       K5(J)=H*F(J)
141   CONTINUE
C
      DO 151 J=1,IN
       CC(J)=CONPOL(J)-8.0D00*K1(J)/2.7D1+2.0D00*K2(J)-
     1     3.544D3*K3(J)/2.565D3+1.859D3*K4(J)/4.104D3-1.1D1*K5(J)/4.0D1
151   CONTINUE
C
      CALL FUNCTN(CC,CONPOL,F,IN)
C
      DO 161 J=1,IN
       K6(J)=H*F(J)
161   CONTINUE
C
C     DETERMINE THE NEW CONCENTRATION OF THE IODINE HYDROLYSIS SPECIES
C     IN THE SUMP POOL AND CHECK ERROR
C
      DO 101 J=1,IN
       CCB(J)=CONPOL(J)+1.6D1*K1(J)/1.35D2+6.656D3*K3(J)/1.2825D4+
     1       2.8561D4*K4(J)/5.643D4-9.0D00*K5(J)/5.0D1+2.0D00*K6(J)/5.5D1
       R(J)=ABS(K1(J)/3.6D2-1.28D2*K3(J)/4.275D3-2.197D3*K4(J)/7.524D4
     1           +K5(J)/5.0D1+2.0D00*K6(J)/5.5D1)/H
       TOL(J)=ABS(CCB(J)*TOLER)
       DELTA(J)=0.84*(TOL(J)/R(J))**0.25
101   CONTINUE
C
      DO 501 J=1,IN
       IF(R(J) .GT. TOL(J))GOTO 901
501   CONTINUE
C
      DO 511 J=1,IN
       CONPOL(J)=CCB(J)
511   CONTINUE
C
C     DETERMINE THE EQUILUBRIUM CONCENTRATION OF EQUATIONS 23, 24 AND
C     25
C
      BB=-1.0D00-(CONPOL(2)+CONPOL(1))*RK4
      C=CONPOL(2)*CONPOL(1)*RK4-CONPOL(7)
      D=-BB/(2.0D00*RK4)
      E=((BB**2.0D00-4.0D00*RK4*C)**0.5D00)/(2.0D00*RK4)
      V=D-E
C
666   IF(V .LT. 1.0D-18 .AND. V .NE. 0.0D00)CALL ITTER(CONPOL,RK4,C,V)
C
      CONPOL(7)=CONPOL(7)+V
      CONPOL(1)=CONPOL(1)-V
      CONPOL(2)=CONPOL(2)-V
C
      IF(IN .EQ. 4)GOTO 601
```

```
C
      RR=CONPOL(6)+CONPOL(5)+RK5
      S=-RK5*CONPOL(3)+CONPOL(6)*CONPOL(5)
      M=(-RR+(RR*RR-4.0D00*S)**0.5)/2.0D00
      CONPOL(5)=CONPOL(5)+M
      GOTO 606
C
601   M=(RK5*CONPOL(3)-CONPOL(6)*CONPOL(5))/(CONPOL(5)+RK5)
C
606   CONPOL(6)=CONPOL(6)+M
      CONPOL(3)=CONPOL(3)-M
C
      IF(IN .EQ. 4)GOTO 616
C
      U=CONPOL(8)*CONPOL(5)-RK6
      VV=CONPOL(8)+CONPOL(5)
      X=(-VV+(VV*VV-4.0D00*U)**0.5)/2.0D00
      CONPOL(5)=CONPOL(5)+X
      CONPOL(8)=CONPOL(8)+X
C
616   PTOLD=PTOLD+H
      DEL=DELTA(1)
C
      IF(IN .EQ. 1)GOTO 906
C
      DO 521 J=2,IN
       IF(DEL .LT. DELTA(J))GOTO 521
       DEL=DELTA(J)
521   CONTINUE
C
      GOTO 906
C
C     DETERMINE NEW STEP SIZE
C
901   DEL=DELTA(J)
C
906   IF(DEL .GT. Q)GOTO 911
      HNEW=Q*H
      GOTO 1001
C
911   IF(DEL .LT. 4.0)GOTO 921
      HNEW=4.0D00*H
      GOTO 1001
C
921   HNEW=DEL*H
C
C     CHECK NEW STEP SIZE WITH MAX AND MIN STEP SIZE
C
1001  IF (HNEW .LT. HMAX)GOTO 931
      HNEW=HMAX
C
931   IF (HNEW .LT. HMIN)GOTO 1112
      LEFT=B-PTOLD-HNEW
C
      IF(LEFT .GT. 0.0)GOTO 5001
      HNEW=B-PTOLD
C
5001  H=HNEW
C
      IF(PTOLD .GE. B)GOTO 998
      GOTO 2
C
C
1112  WRITE(40,21)HNEW
998   RETURN
      END
```

```
C***********************************************************************
C
C     SUBROUTINE FUNCTN
C
C     THIS SUBROUTINE CONTAINS THE DIFFERENTIAL EQUATIONS (KINETIC RATE
C     EQUATIONS) TO BE INTEGRATED.  THIS SUBROUTINE IS CALLED FROM THE
C     RUNGE-KUTTA-FELHBURG INTEGRATION ROUTINE IN THE KINETIC, DROP,
C     SPRAY AND WALL-SPRAY MODELS.
C
C***********************************************************************
C
      SUBROUTINE FUNCTN (W,WOLD,F,IN)
C
      IMPLICIT DOUBLE PRECISION(A-H,K-Z)
      IMPLICIT INTEGER(I-J)
C
      DIMENSION W(8),WOLD(8),F(7)
C
      IF(IN .EQ. 5)GOTO 5
C
      W(5)=WOLD(5)
5     W(6)=WOLD(6)
C
      RK1=3.0D00
      RKR1=4.4D12
      RK20=2.5D02
      RK21=1.2D02
      RKR2=3.0D08
      RKP3=9.35D-8
C
      R1=RK1*W(1)
      RR1=RKR1*W(2)*W(3)*W(5)
      R20=RK20*W(3)**2.0D00
      R21=RK21*W(3)*W(6)
      RR2=RKR2*W(4)*W(2)**2.0D00*W(5)**2.0D00
      RP3=RKP3*W(5)*W(2)
C
      F(1)=-R1+RR1+5.0D-1*RP3
      F(2)=R1-RR1+2.0D00*(R20+R21)/3.0D00-2.0D00*RR2-RP3
      F(3)=R1-RR1-R20-R21+3.0D00*RR2
      F(4)=(R20+R21)/3.0D00-RR2
C
      IF (IN .EQ. 5)GOTO 10
C
      F(5)=0.0D00
      GOTO 11
C
10    F(5)=R1-RR1+R20+R21-3.0D00*RR2-4.0D00*RP3
C
11    F(6)=0.0D00
      F(7)=0.0D00
C
      RETURN
C
      END
```

```
C*********************************************************************
C
C     SUBROUTINE ITTER
C
C     THIS SUBROUTINE FINDS THE ROOT TO THE QUADRATIC EQUILIBRIUM
C     EQUATION FOR THE FORMATION REACTION OF TRI-IODIDE, I3- (EQUATION
C     23).  A SECANT METHOD IS THE ROUTINE USED TO FIND THE ROOT.  THIS
C     METHOD IS CALLED WHENEVER THE QUADRATIC FORMULA RESULTS IN LESS
C     THAN APPROXIMATELY THREE SIGNIFICANT FIGURES.  THIS SUBROUTINE
C     IS CALLED BY THE PROGRAMS KINETIC, DROP, SPRAY AND WALL-SPRAY.
C
C*********************************************************************
C
      SUBROUTINE ITTER(WOLD,RK4,C,V)
C
      IMPLICIT DOUBLE PRECISION (A-H,L-Z)
      IMPLICIT INTEGER (I-K)
C
      DIMENSION WOLD(7),W(7)
C
      P0=1.0D-16
      P1=1.0D-18
C
      Q0=C-RK4*P0*P0-P0*RK4*(WOLD(1)+WOLD(2))-P0
5     Q1=C-RK4*P1*P1-P1*RK4*(WOLD(1)+WOLD(2))-P1
C
      NEW=P1-Q1*(P1-P0)/(Q1-Q0)
C
      CHECK=ABS(NEW-P1)/P1
C
11    IF (CHECK .LT. 1.0D-4) GOTO 10
C
      P0=P1
      Q0=Q1
      P1=NEW
      GOTO 5
C
10    V=NEW
C
      RETURN
C
      END
```

Wall-Spray Model sample input:

A = 0.0

B = DURTM = 10

HMIN = 1.0×10^{-10}

HMAX = 1.0×10^{2}

IN = 4

TOLER = 1.0×10^{-3}

TEMPL = 298

TEMPG = 298

DIAM = 0.1

SAD = 0.1

CI2G = 1.0×10^{-7}

CI2SP = 0.0

CISP = 0.0

CHOISP = 0.0

COISP = 0.0

CHSP = 1.0×10^{-9}

CIO3SP = 0.0

CI3SP = 0.0

PRESS = 1.0

CDIAM = 3.13

HEIGHT = 15.4

FLRAT = 37.0

WFRAC = 0.05

WHT = 3.3

```
AT A TEMPERTURE OF THE GAS 298.00 DEGRESS KELVIN
THE VISCOSITY OF THE LIQUID (CP)=  0.8972334E+00
THE VISCOSITY OF THE GAS (CP) =  0.1838378E-01
THE PARTITION COEFFICIENT IS =  0.8683416E+02
THE DENSITY OF THE LIQUID (GMS/CC) =  0.9969160E+00
THE DENSITY OF THE GAS (GMS/CC) =  0.1182949E-02
THE DIFFUSION COEFFICIENT FOR THE GAS (SQ CM/SEC)=  0.8040764E-01
THE DIFFUSION COEFFICIENT FOR THE LIQUID (SQ CM/SEC)=  0.1298637E-04
THE GAS-SIDE MASS TRANSFER COEFFICIENT (CM/SEC)=  0.1127948E+02
THE LIQUID-SIDE MASS TRANSFER COEFFICIENT (CM/SEC)=  0.2553658E+00
THE OVERALL LIQUID-SIDE MASS TRANSFER COEFFICIENT (CM/SEC)=  0.8610024E-01
THE VOLUME FOR ONE DROP (LITERS)=  0.5236000E-06
THE SURFACE AREA FOR ONE DROP (SQ CM)=  0.3141600E-01
THE EXPOSURE TIME FOR THE DROP IS (SEC)=  0.3904862E+01
THE REYNOLDS NUMBER FOR THE DROP =  0.2537734E+03
THE TERMINAL VELOCITY OF THE DROP (CM/SEC) =  0.3943801E+03
THE NUMBER OF DROPS IN THE CONTAINMENT IS  0.4723222E+07
THE DROP FLUX (NUMBER OF DROPS/SQ CM MIN) =  0.8247353E+03
THE CONTAINMENT VOLUME (LITERS) =  0.1355158E+06
THE NUMBER OF OUTER LOOPS =    154
THE INITIAL CONCENTRATION IN THE GAS OF  0.1000000E-06 (MOLES/LITER)
THE DURATION OF THE SPRAY (MIN)    0.1000000E+02
THE VOLUME OF LIQUID SPRAYED (LITERS)    0.3800000E+03
AND A SPRAY FLOW RATE OF    0.3800000E+02 (LITERS/MIN)
THE INITIAL CONCENTRATION OF THE LIQUID (MOLES/LITER) :
                    I2 =   0.0000000E+00
                    I- =   0.0000000E+00
                   HOI =   0.0000000E+00
                  IO3- =   0.0000000E+00
                    H+ =   0.1000000E-08
                   IO- =   0.0000000E+00
                   I3- =   0.0000000E+00
THE FINAL CONCENTRATION OF IODINE (I2) IN THE GAS IS   0.1633250E-07 (MOLES/LITER)
THE NUMBER OF MOLES OF IODINE (I2) REMOVED IS =  0.1133827E-01
THE NUMBER OF GRAMS OF IODINE REMOVES IS =  0.2877756E+01
THE FINAL CONCENTRATION OF THE LIQUID IS (MOLES/LITER) :
                    I2 =   0.5854641E-06
                    I- =   0.4341304E-04
                   HOI =   0.9187987E-05
                  IO3- =   0.6860263E-05
                    H+ =   0.1000000E-08
                   IO- =   0.4969644E-10
                   I3- =   0.7630769E-07
```

FOR50

DAT

File: DSKB:FOR50.DAT[6452,232] Created: 09-Dec-84 17:27:00 <055> Printed: 09-Dec-84 17:32:29
QUEUE Switches: /FILE:FORT /COPIES:1 /SPACING:1 /LIMIT:276

CONCENTRATION OF THE DROPS

#	TIME	I2	I-	HOI	IO3-	H+	IO-	I3-
0	.0000000D+00	.0000000D+00	.0000000D+00	.0000000D+00	.0000000D+00	.1000000D-08	.0000000D+00	.0000000D+00
1	.6508103D-01	.6819839D-05	.5374871D-04	.5119192D-04	.3311030D-06	.1000000D-08	.1172053D-05	.2707823D-06
2	.1301621D+00	.6735996D-05	.5326789D-04	.5074677D-04	.3248626D-06	.1000000D-08	.1161862D-05	.2650607D-06
3	.1952431D+00	.6653073D-05	.5278990D-04	.5030400D-04	.3187241D-06	.1000000D-08	.1151724D-05	.2594485D-06
4	.2603241D+00	.6571062D-05	.5231475D-04	.4986362D-04	.3126857D-06	.1000000D-08	.1141642D-05	.2539439D-06
5	.3254052D+00	.6489957D-05	.5184244D-04	.4942564D-04	.3067484D-06	.1000000D-08	.1131614D-05	.2485452D-06
6	.3904862D+00	.6409749D-05	.5137298D-04	.4899006D-04	.3009049D-06	.1000000D-08	.1121641D-05	.2432506D-06
7	.4555672D+00	.6330432D-05	.5090636D-04	.4855690D-04	.2951559D-06	.1000000D-08	.1111724D-05	.2380584D-06
8	.5206483D+00	.6251998D-05	.5044260D-04	.4812615D-04	.2895104D-06	.1000000D-08	.1101862D-05	.2329670D-06
9	.5857293D+00	.6174440D-05	.4998169D-04	.4769784D-04	.2839549D-06	.1000000D-08	.1092055D-05	.2279747D-06
10	.6508103D+00	.6097751D-05	.4952364D-04	.4727195D-04	.2784924D-06	.1000000D-08	.1082305D-05	.2230799D-06
11	.7158914D+00	.6021924D-05	.4906845D-04	.4684851D-04	.2731216D-06	.1000000D-08	.1072610D-05	.2182809D-06
12	.7809724D+00	.5946951D-05	.4861612D-04	.4642752D-04	.2678413D-06	.1000000D-08	.1062971D-05	.2135761D-06
13	.8460534D+00	.5872825D-05	.4816665D-04	.4600898D-04	.2626502D-06	.1000000D-08	.1053388D-05	.2089641D-06
14	.9111344D+00	.5799539D-05	.4772005D-04	.4559289D-04	.2575473D-06	.1000000D-08	.1043862D-05	.2044431D-06
15	.9762155D+00	.5727086D-05	.4727631D-04	.4517928D-04	.2525314D-06	.1000000D-08	.1034392D-05	.2000117D-06
16	.1041297D+01	.5655458D-05	.4683545D-04	.4476813D-04	.2476012D-06	.1000000D-08	.1024979D-05	.1956683D-06
17	.1106378D+01	.5584648D-05	.4639745D-04	.4435946D-04	.2427557D-06	.1000000D-08	.1015622D-05	.1914115D-06
18	.1171459D+01	.5514650D-05	.4596231D-04	.4395326D-04	.2379937D-06	.1000000D-08	.1006322D-05	.1872397D-06
19	.1236540D+01	.5445455D-05	.4553005D-04	.4354955D-04	.2333139D-06	.1000000D-08	.9970792D-06	.1831515D-06
20	.1301621D+01	.5377058D-05	.4510065D-04	.4314833D-04	.2287154D-06	.1000000D-08	.9878931D-06	.1791454D-06
21	.1366702D+01	.5309450D-05	.4467413D-04	.4274960D-04	.2241965D-06	.1000000D-08	.9787640D-06	.1752200D-06
22	.1431783D+01	.5242625D-05	.4425047D-04	.4235336D-04	.2197574D-06	.1000000D-08	.9696921D-06	.1713739D-06
23	.1496864D+01	.5176575D-05	.4382968D-04	.4195963D-04	.2153958D-06	.1000000D-08	.9606774D-06	.1676057D-06
24	.1561945D+01	.5111294D-05	.4341175D-04	.4156839D-04	.2111106D-06	.1000000D-08	.9517199D-06	.1639141D-06
25	.1627026D+01	.5046774D-05	.4299669D-04	.4117966D-04	.2069016D-06	.1000000D-08	.9428197D-06	.1602976D-06
26	.1692107D+01	.4983008D-05	.4258449D-04	.4079343D-04	.2027669D-06	.1000000D-08	.9339770D-06	.1567549D-06
27	.1757188D+01	.4919990D-05	.4217515D-04	.4040971D-04	.1987057D-06	.1000000D-08	.9251916D-06	.1532847D-06
28	.1822269D+01	.4857712D-05	.4176867D-04	.4002850D-04	.1947170D-06	.1000000D-08	.9164637D-06	.1498858D-06
29	.1887350D+01	.4796168D-05	.4136504D-04	.3964980D-04	.1907995D-06	.1000000D-08	.9077933D-06	.1465568D-06
30	.1952431D+01	.4735350D-05	.4096427D-04	.3927362D-04	.1869527D-06	.1000000D-08	.8991805D-06	.1432964D-06
31	.2017512D+01	.4675251D-05	.4056634D-04	.3889995D-04	.1831750D-06	.1000000D-08	.8906252D-06	.1401035D-06
32	.2082593D+01	.4615865D-05	.4017127D-04	.3852879D-04	.1794657D-06	.1000000D-08	.8821274D-06	.1369767D-06
33	.2147674D+01	.4557185D-05	.3977904D-04	.3816015D-04	.1758236D-06	.1000000D-08	.8736872D-06	.1339149D-06
34	.2212755D+01	.4499203D-05	.3938964D-04	.3779402D-04	.1722477D-06	.1000000D-08	.8653046D-06	.1309169D-06

35	.2277036D+01	.4441914D-05	.3900309D-04	.3743040D-04	.1687372D-06	.1000000D-08	.8569795D-06	.1279815D-06
36	.2342917D+01	.4385310D-05	.3861936D-04	.3706930D-04	.1652909D-06	.1000000D-08	.8487120D-06	.1251075D-06
37	.2407998D+01	.4329384D-05	.3823846D-04	.3671071D-04	.1619080D-06	.1000000D-08	.8405020D-06	.1222939D-06
38	.2473079D+01	.4274131D-05	.3786038D-04	.3635663D-04	.1585874D-06	.1000000D-08	.8323495D-06	.1195393D-06
39	.2538160D+01	.4219542D-05	.3748512D-04	.3600107D-04	.1553282D-06	.1000000D-08	.8242545D-06	.1168429D-06
40	.2603241D+01	.4165612D-05	.3711267D-04	.3565001D-04	.1521294D-06	.1000000D-08	.8162169D-06	.1142034D-06
41	.2668322D+01	.4112333D-05	.3674303D-04	.3530146D-04	.1489901D-06	.1000000D-08	.8082368D-06	.1116198D-06
42	.2733403D+01	.4059700D-05	.3637618D-04	.3495541D-04	.1459094D-06	.1000000D-08	.8003140D-06	.1090911D-06
43	.2798484D+01	.4007705D-05	.3601214D-04	.3461187D-04	.1428864D-06	.1000000D-08	.7924484D-06	.1066161D-06
44	.2863565D+01	.3956342D-05	.3565087D-04	.3427083D-04	.1399201D-06	.1000000D-08	.7846402D-06	.1041939D-06
45	.2928646D+01	.3905605D-05	.3529240D-04	.3393228D-04	.1370097D-06	.1000000D-08	.7768891D-06	.1018234D-06
46	.2993727D+01	.3855487D-05	.3493669D-04	.3359623D-04	.1341542D-06	.1000000D-08	.7691950D-06	.9950368D-07
47	.3058808D+01	.3805982D-05	.3458376D-04	.3326267D-04	.1313528D-06	.1000000D-08	.7615580D-06	.9723373D-07
48	.3123890D+01	.3757083D-05	.3423358D-04	.3293159D-04	.1286046D-06	.1000000D-08	.7539780D-06	.9501259D-07
49	.3188971D+01	.3708783D-05	.3388616D-04	.3260300D-04	.1259088D-06	.1000000D-08	.7464548D-06	.9283931D-07
50	.3254052D+01	.3661078D-05	.3354148D-04	.3227688D-04	.1232645D-06	.1000000D-08	.7389883D-06	.9071295D-07
51	.3319133D+01	.3613959D-05	.3319954D-04	.3195324D-04	.1206707D-06	.1000000D-08	.7315785D-06	.8863260D-07
52	.3384214D+01	.3567422D-05	.3286034D-04	.3163207D-04	.1181270D-06	.1000000D-08	.7242252D-06	.8659735D-07
53	.3449295D+01	.3521460D-05	.3252385D-04	.3131337D-04	.1156322D-06	.1000000D-08	.7169283D-06	.8460632D-07
54	.3514376D+01	.3476066D-05	.3219008D-04	.3099712D-04	.1131856D-06	.1000000D-08	.7096878D-06	.8265862D-07
55	.3579457D+01	.3431234D-05	.3185901D-04	.3068333D-04	.1107864D-06	.1000000D-08	.7025034D-06	.8075340D-07
56	.3644518D+01	.3386959D-05	.3153064D-04	.3037199D-04	.1084336D-06	.1000000D-08	.6953751D-06	.7888981D-07
57	.3709619D+01	.3343235D-05	.3120496D-04	.3006309D-04	.1061271D-06	.1000000D-08	.6883028D-06	.7706702D-07
58	.3774700D+01	.3300055D-05	.3088195D-04	.2975662D-04	.1038654D-06	.1000000D-08	.6812862D-06	.7528422D-07
59	.3839791D+01	.3257813D-05	.3056161D-04	.2945259D-04	.1016489D-06	.1000000D-08	.6743753D-06	.7350600D-07
60	.3904862D+01	.3215303D-05	.3024393D-04	.2915098D-04	.9947415D-07	.1000000D-08	.6674198D-06	.7183537D-07
61	.3969943D+01	.3173721D-05	.2992890D-04	.2885179D-04	.9734311D-07	.1000000D-08	.6605697D-06	.7016776D-07
62	.4035024D+01	.3132658D-05	.2961651D-04	.2855501D-04	.9525414D-07	.1000000D-08	.6537748D-06	.6853700D-07
63	.4100105D+01	.3092111D-05	.2930675D-04	.2826063D-04	.9320652D-07	.1000000D-08	.6470349D-06	.6694234D-07
64	.4165186D+01	.3052073D-05	.2899961D-04	.2796864D-04	.9119953D-07	.1000000D-08	.6403499D-06	.6538305D-07
65	.4230267D+01	.3012539D-05	.2869507D-04	.2767905D-04	.8923248D-07	.1000000D-08	.6337196D-06	.6385840D-07
66	.4295348D+01	.2973502D-05	.2839313D-04	.2739184D-04	.8730467D-07	.1000000D-08	.6271437D-06	.6236769D-07
67	.4360429D+01	.2934957D-05	.2809378D-04	.2710699D-04	.8541534D-07	.1000000D-08	.6206222D-06	.6091021D-07
68	.4425510D+01	.2896899D-05	.2779701D-04	.2682452D-04	.8356392D-07	.1000000D-08	.6141548D-06	.5948528D-07
69	.4490591D+01	.2859322D-05	.2750280D-04	.2654440D-04	.8174976D-07	.1000000D-08	.6077414D-06	.5809222D-07
70	.4555672D+01	.2822220D-05	.2721114D-04	.2626663D-04	.7997202D-07	.1000000D-08	.6013818D-06	.5673038D-07
71	.4620753D+01	.2785588D-05	.2692202D-04	.2599119D-04	.7823024D-07	.1000000D-08	.5950756D-06	.5539910D-07
72	.4685834D+01	.2749421D-05	.2663544D-04	.2571809D-04	.7652376D-07	.1000000D-08	.5888229D-06	.5409775D-07
73	.4750915D+01	.2713713D-05	.2635137D-04	.2544731D-04	.7485178D-07	.1000000D-08	.5826233D-06	.5282570D-07
74	.4815996D+01	.2678460D-05	.2606981D-04	.2517884D-04	.7321387D-07	.1000000D-08	.5764767D-06	.5158234D-07
75	.4881077D+01	.2643654D-05	.2579074D-04	.2491268D-04	.7160933D-07	.1000000D-08	.5703827D-06	.5036706D-07
76	.4946158D+01	.2609293D-05	.2551416D-04	.2464881D-04	.7003757D-07	.1000000D-08	.5643413D-06	.4917927D-07
77	.5011219D+01	.2575369D-05	.2524004D-04	.2438722D-04	.6849806D-07	.1000000D-08	.5583522D-06	.4801840D-07
78	.5076320D+01	.2541878D-05	.2496839D-04	.2412791D-04	.6699002D-07	.1000000D-08	.5524152D-06	.4688386D-07
79	.5141402D+01	.2508816D-05	.2469918D-04	.2387086D-04	.6551306D-07	.1000000D-08	.5465300D-06	.4577511D-07
80	.5206483D+01	.2476176D-05	.2443240D-04	.2361606D-04	.6406654D-07	.1000000D-08	.5406964D-06	.4469159D-07
81	.5271564D+01	.2443955D-05	.2416804D-04	.2336351D-04	.6264990D-07	.1000000D-08	.5349141D-06	.4363276D-07
82	.5336645D+01	.2412146D-05	.2390609D-04	.2311320D-04	.6126260D-07	.1000000D-08	.5291831D-06	.4259810D-07
83	.5401726D+01	.2380745D-05	.2364654D-04	.2286510D-04	.5990408D-07	.1000000D-08	.5235029D-06	.4158709D-07
84	.5466807D+01	.2349747D-05	.2338936D-04	.2261922D-04	.5857381D-07	.1000000D-08	.5178734D-06	.4059922D-07
85	.5531888D+01	.2319188D-05	.2313456D-04	.2237554D-04	.5727126D-07	.1000000D-08	.5122942D-06	.3963399D-07
86	.5596969D+01	.2288942D-05	.2288210D-04	.2213405D-04	.5599591D-07	.1000000D-08	.5067653D-06	.3869091D-07
87	.5662050D+01	.2259125D-05	.2263199D-04	.2189474D-04	.5474725D-07	.1000000D-08	.5012862D-06	.3776950D-07
88	.5727131D+01	.2229693D-05	.2238421D-04	.2165760D-04	.5352477D-07	.1000000D-08	.4958568D-06	.3686930D-07
89	.5792212D+01	.2200639D-05	.2213874D-04	.2142262D-04	.5232797D-07	.1000000D-08	.4904768D-06	.3598984D-07
90	.5857293D+01	.2171961D-05	.2189556D-04	.2118978D-04	.5115638D-07	.1000000D-08	.4851459D-06	.3513067D-07
91	.5922374D+01	.2143652D-05	.2165470D-04	.2095908D-04	.5000949D-07	.1000000D-08	.4798640D-06	.3429135D-07
92	.5987455D+01	.2115710D-05	.2141609D-04	.2073050D-04	.4888684D-07	.1000000D-08	.4746306D-06	.3347145D-07
93	.6052536D+01	.2088129D-05	.2117975D-04	.2050403D-04	.4778800D-07	.1000000D-08	.4694455D-06	.3267053D-07
94	.6117617D+01	.2060505D-05	.2094565D-04	.2027966D-04	.4671245D-07	.1000000D-08	.4643086D-06	.3188818D-07
95	.6182698D+01	.2034033D-05	.2071378D-04	.2005739D-04	.4565978D-07	.1000000D-08	.4592194D-06	.3112400D-07
96	.6247779D+01	.2007509D-05	.2048413D-04	.1983718D-04	.4462953D-07	.1000000D-08	.4541778D-06	.3037758D-07
97	.6312860D+01	.1981329D-05	.2025668D-04	.1961908D-04	.4362127D-07	.1000000D-08	.4491835D-06	.2964853D-07
98	.6377941D+01	.1955489D-05	.2003143D-04	.1940296D-04	.4263457D-07	.1000000D-08	.4442361D-06	.2893646D-07
99	.6443022D+01	.1929985D-05	.1980835D-04	.1918891D-04	.4166901D-07	.1000000D-08	.4393354D-06	.2824101D-07
100	.6508103D+01	.1904811D-05	.1958743D-04	.1897689D-04	.4072417D-07	.1000000D-08	.4344812D-06	.2756179D-07
101	.6573184D+01	.1879965D-05	.1936866D-04	.1876688D-04	.3979965D-07	.1000000D-08	.4296731D-06	.2689846D-07
102	.6638265D+01	.1855441D-05	.1915202D-04	.1855888D-04	.3889504D-07	.1000000D-08	.4249108D-06	.2625064D-07
103	.6703346D+01	.1831237D-05	.1893750D-04	.1835287D-04	.3800995D-07	.1000000D-08	.4201942D-06	.2561801D-07
104	.6768427D+01	.1807388D-05	.1872568D-04	.1814884D-04	.3714400D-07	.1000000D-08	.4155228D-06	.2500021D-07
105	.6833508D+01	.1783770D-05	.1851476D-04	.1794677D-04	.3629679D-07	.1000000D-08	.4108964D-06	.2439692D-07
106	.6898589D+01	.1760499D-05	.1830651D-04	.1774666D-04	.3546757D-07	.1000000D-08	.4063148D-06	.2380781D-07
107	.6963670D+01	.1737531D-05	.1810032D-04	.1754849D-04	.3465715D-07	.1000000D-08	.4017775D-06	.2323255D-07
108	.7028751D+01	.1714863D-05	.1789618D-04	.1735224D-04	.3386358D-07	.1000000D-08	.3972844D-06	.2267085D-07
109	.7093832D+01	.1692491D-05	.1769407D-04	.1715791D-04	.3308811D-07	.1000000D-08	.3928352D-06	.2212239D-07
110	.7158914D+01	.1670410D-05	.1749397D-04	.1696548D-04	.3232918D-07	.1000000D-08	.3884295D-06	.2158687D-07
111	.7223995D+01	.1648618D-05	.1729588D-04	.1677494D-04	.3158665D-07	.1000000D-08	.3840670D-06	.2106400D-07
112	.7289076D+01	.1627111D-05	.1709978D-04	.1658628D-04	.3086079D-07	.1000000D-08	.3797476D-06	.2055350D-07
113	.7354157D+01	.1605884D-05	.1690565D-04	.1639948D-04	.3015064D-07	.1000000D-08	.3754708D-06	.2005507D-07
114	.7419238D+01	.1584935D-05	.1671348D-04	.1621454D-04	.2945614D-07	.1000000D-08	.3712363D-06	.1956846D-07
115	.7484319D+01	.1564260D-05	.1652326D-04	.1603143D-04	.2877691D-07	.1000000D-08	.3670440D-06	.1909338D-07
116	.7549400D+01	.1543855D-05	.1633497D-04	.1585014D-04	.2811268D-07	.1000000D-08	.3628934D-06	.1862957D-07
117	.7614481D+01	.1523717D-05	.1614859D-04	.1567067D-04	.2746306D-07	.1000000D-08	.3587843D-06	.1817679D-07
118	.7679562D+01	.1503843D-05	.1596411D-04	.1549299D-04	.2682783D-07	.1000000D-08	.3547164D-06	.1773477D-07
119	.7744643D+01	.1484229D-05	.1578152D-04	.1531710D-04	.2620673D-07	.1000000D-08	.3506894D-06	.1730326D-07
120	.7809724D+01	.1464872D-05	.1560081D-04	.1514299D-04	.2559933D-07	.1000000D-08	.3467030D-06	.1688204D-07
121	.7874805D+01	.1445768D-05	.1542195D-04	.1497063D-04	.2500550D-07	.1000000D-08	.3427568D-06	.1647085D-07
122	.7939886D+01	.1426915D-05	.1524493D-04	.1480002D-04	.2442485D-07	.1000000D-08	.3388507D-06	.1606947D-07
123	.8004367D+01	.1408309D-05	.1506974D-04	.1463115D-04	.2385713D-07	.1000000D-08	.3349843D-06	.1567768D-07
124	.8070048D+01	.1389946D-05	.1489637D-04	.1446400D-04	.2330265D-07	.1000000D-08	.3311572D-06	.1529525D-07
125	.8135129D+01	.1371825D-05	.1472879D-04	.1429055D-04	.2275948D-07	.1000000D-08	.3273693D-06	.1492196D-07

126	.8200210D+01	.1353941D-05	.1455500D-04	.1413480D-04	.2222895D-07	.1000000D-08	.3236201D-06	.1455761D-07
127	.8265291D+01	.1336291D-05	.1438659D-04	.1357273D-04	.2171034D-07	.1000000D-08	.3199095D-06	.1420199D-07
128	.8330372D+01	.1318873D-05	.1422072D-04	.1381233D-04	.2120337D-07	.1000000D-08	.3162370D-06	.1385488D-07
129	.8395453D+01	.1301684D-05	.1405620D-04	.1365358D-04	.2070779D-07	.1000000D-08	.3126025D-06	.1351611D-07
130	.8460534D+01	.1284720D-05	.1389341D-04	.1349648D-04	.2022336D-07	.1000000D-08	.3090056D-06	.1318547D-07
131	.8525615D+01	.1267979D-05	.1373233D-04	.1334100D-04	.1974985D-07	.1000000D-08	.3054460D-06	.1286277D-07
132	.8590696D+01	.1251457D-05	.1357296D-04	.1318714D-04	.1928702D-07	.1000000D-08	.3019234D-06	.1254783D-07
133	.8655777D+01	.1235153D-05	.1341526D-04	.1303489D-04	.1883465D-07	.1000000D-08	.2984375D-06	.1224047D-07
134	.8720858D+01	.1219062D-05	.1325924D-04	.1288423D-04	.1839251D-07	.1000000D-08	.2949880D-06	.1194050D-07
135	.8785939D+01	.1203183D-05	.1310487D-04	.1273514D-04	.1796038D-07	.1000000D-08	.2915746D-06	.1164776D-07
136	.8851020D+01	.1187512D-05	.1295215D-04	.1258762D-04	.1753806D-07	.1000000D-08	.2881971D-06	.1136208D-07
137	.8916101D+01	.1172047D-05	.1280105D-04	.1244165D-04	.1712532D-07	.1000000D-08	.2848551D-06	.1108330D-07
138	.8981182D+01	.1156786D-05	.1265157D-04	.1229722D-04	.1672157D-07	.1000000D-08	.2815484D-06	.1081124D-07
139	.9046263D+01	.1141724D-05	.1250369D-04	.1215432D-04	.1632780D-07	.1000000D-08	.2782766D-06	.1054575D-07
140	.9111344D+01	.1126861D-05	.1235740D-04	.1201293D-04	.1594261D-07	.1000000D-08	.2750394D-06	.1028668D-07
141	.9176425D+01	.1112192D-05	.1221268D-04	.1187304D-04	.1556621D-07	.1000000D-08	.2718367D-06	.1003388D-07
142	.9241507D+01	.1097717D-05	.1206952D-04	.1173464D-04	.1519841D-07	.1000000D-08	.2686680D-06	.9787196D-08
143	.9306588D+01	.1083431D-05	.1192790D-04	.1159772D-04	.1483902D-07	.1000000D-08	.2655330D-06	.9546485D-08
144	.9371669D+01	.1069334D-05	.1178782D-04	.1146226D-04	.1448787D-07	.1000000D-08	.2624316D-06	.9311607D-08
145	.9436750D+01	.1055421D-05	.1164925D-04	.1132825D-04	.1414476D-07	.1000000D-08	.2593633D-06	.9082425D-08
146	.9501831D+01	.1041691D-05	.1151219D-04	.1119567D-04	.1380952D-07	.1000000D-08	.2563280D-06	.8858802D-08
147	.9566912D+01	.1028142D-05	.1137662D-04	.1106452D-04	.1348195D-07	.1000000D-08	.2533253D-06	.8640607D-08
148	.9631993D+01	.1014770D-05	.1124252D-04	.1093479D-04	.1316199D-07	.1000000D-08	.2503550D-06	.8427713D-08
149	.9697074D+01	.1001575D-05	.1110989D-04	.1080645D-04	.1284937D-07	.1000000D-08	.2474167D-06	.8219992D-08
150	.9762155D+01	.9885524D-06	.1097871D-04	.1067950D-04	.1254394D-07	.1000000D-08	.2445102D-06	.8017321D-08
151	.9827236D+01	.9757011D-06	.1084897D-04	.1055393D-04	.1224557D-07	.1000000D-08	.2416352D-06	.7819582D-08
152	.9892317D+01	.9630187D-06	.1072066D-04	.1042972D-04	.1195409D-07	.1000000D-08	.2387914D-06	.7626656D-08
153	.9957398D+01	.9505028D-06	.1059375D-04	.1030686D-04	.1166935D-07	.1000000D-08	.2359785D-06	.7438428D-08
154	.1002248D+02	.9381514D-06	.1046824D-04	.1018534D-04	.1139120D-07	.1000000D-08	.2331963D-06	.7254787D-08

FOR51

DAT

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QUEUE Switches: /FILE:FORT /COPIES:1 /SPACING:1 /LIMIT:273

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0.1952431D+00	0.1433961D-03	0.9679560D-07	0.4342469D-03
0.2603241D+00	0.1420552D-03	0.9574734D-07	0.5763022D-03
0.3254052D+00	0.1407233D-03	0.9470892D-07	0.7170254D-03
0.3904862D+00	0.1394003D-03	0.3368025D-07	0.8564258D-03
0.4555672D+00	0.1380864D-03	0.9266129D-07	0.9945121D-03
0.5206483D+00	0.1367813D-03	0.9165195D-07	0.1131293D-02
0.5857293D+00	0.1354852D-03	0.9065217D-07	0.1266779D-02
0.6508103D+00	0.1341980D-03	0.8966190D-07	0.1400977D-02
0.7158914D+00	0.1329198D-03	0.8868105D-07	0.1533897D-02
0.7809724D+00	0.1316504D-03	0.8770958D-07	0.1665547D-02
0.8460534D+00	0.1303900D-03	0.8674740D-07	0.1795937D-02
0.9111344D+00	0.1291384D-03	0.8579446D-07	0.1925075D-02
0.9762155D+00	0.1278957D-03	0.8485069D-07	0.2052971D-02
0.1041297D+01	0.1266618D-03	0.8391603D-07	0.2179633D-02
0.1106378D+01	0.1254368D-03	0.8299040D-07	0.2305070D-02
0.1171459D+01	0.1242206D-03	0.8207376D-07	0.2429290D-02
0.1236540D+01	0.1230132D-03	0.8116601D-07	0.2552303D-02
0.1301621D+01	0.1218146D-03	0.8026712D-07	0.2674118D-02
0.1366702D+01	0.1206247D-03	0.7937700D-07	0.2794743D-02
0.1431783D+01	0.1194436D-03	0.7849560D-07	0.2914186D-02
0.1496864D+01	0.1182713D-03	0.7762286D-07	0.3032458D-02
0.1561945D+01	0.1171076D-03	0.7675869D-07	0.3149565D-02
0.1627026D+01	0.1159527D-03	0.7590305D-07	0.3265518D-02
0.1692107D+01	0.1148064D-03	0.7505587D-07	0.3380324D-02
0.1757188D+01	0.1136688D-03	0.7421709D-07	0.3493993D-02
0.1822269D+01	0.1125398D-03	0.7338663D-07	0.3606533D-02
0.1887350D+01	0.1114194D-03	0.7256445D-07	0.3717952D-02
0.1952431D+01	0.1103076D-03	0.7175046D-07	0.3828260D-02
0.2017512D+01	0.1092043D-03	0.7094462D-07	0.3937464D-02
0.2082593D+01	0.1081096D-03	0.7014686D-07	0.4045574D-02
0.2147674D+01	0.1070234D-03	0.6935711D-07	0.4152597D-02
0.2212755D+01	0.1059457D-03	0.6857531D-07	0.4258543D-02
0.2277836D+01	0.1048765D-03	0.6780141D-07	0.4363419D-02
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0.2407998D+01	0.1027633D-03	0.6627702D-07	0.4569998D-02
0.2473079D+01	0.1017192D-03	0.6552641D-07	0.4671717D-02
0.2538160D+01	0.1006836D-03	0.6478345D-07	0.4772401D-02
0.2603241D+01	0.9965626D-04	0.6404806D-07	0.4872057D-02
0.2668322D+01	0.9863723D-04	0.6332020D-07	0.4970694D-02
0.2733403D+01	0.9762646D-04	0.6259579D-07	0.5068321D-02
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0.2863565D+01	0.9562962D-04	0.6118111D-07	0.5260575D-02
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0.3319133D+01	0.8889663D-04	0.5644182D-07	0.5902824D-02
0.3384214D+01	0.8796685D-04	0.5579269D-07	0.5990791D-02
0.3449295D+01	0.8704498D-04	0.5515037D-07	0.6077836D-02
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0.3644538D+01	0.8432653D-04	0.5326363D-07	0.6333518D-02
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0.3774700D+01	0.8255117D-04	0.5203876D-07	0.6499507D-02
0.3839781D+01	0.8167806D-04	0.5143604D-07	0.6581185D-02
0.3904862D+01	0.8081062D-04	0.5083973D-07	0.6661996D-02
0.3969981D+01	0.7995081D-04	0.5028575D-07	0.6781987D-02
0.4035024D+01	0.7909859D-04	0.4966607D-07	0.6821045D-02
0.4100105D+01	0.7825392D-04	0.4908861D-07	0.6899299D-02
0.4155186D+01	0.7741677D-04	0.4851734D-07	0.6976716D-02
0.4230267D+01	0.7658710D-04	0.4795219D-07	0.7053303D-02
0.4295348D+01	0.7576487D-04	0.4739310D-07	0.7129068D-02
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0.4815996D+01	0.6945002D-04	0.4313236D-07	0.7706466D-02
0.4881077D+01	0.6869294D-04	0.4262546D-07	0.7775159D-02
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0.5141402D+01	0.6573455D-04	0.4065269D-07	0.8042500D-02
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0.5466807D+01	0.6219077D-04	0.3830630D-07	0.8360474D-02
0.5531888D+01	0.6150215D-04	0.3785246D-07	0.8421976D-02
0.5596969D+01	0.6082014D-04	0.3740366D-07	0.8482796D-02
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0.5727131D+01	0.5947579D-04	0.3652095D-07	0.8602417D-02
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0.6182698D+01	0.5497247D-04	0.3358299D-07	0.9000557D-02
0.6247779D+01	0.5435420D-04	0.3318190D-07	0.9054911D-02
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0.7744643D+01	0.4173790D-04	0.2511602D-07	0.1014797D-01
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0.8981182D+01	0.3338708D-04	0.1990029D-07	0.1085478D-01
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0.9306588D+01	0.3146152D-04	0.1871138D-07	0.1101590D-01
0.9371669D+01	0.3108901D-04	0.1848196D-07	0.1104699D-01
0.9436750D+01	0.3072060D-04	0.1825527D-07	0.1107771D-01
0.9501831D+01	0.3035626D-04	0.1803126D-07	0.1110806D-01
0.9566912D+01	0.2999596D-04	0.1780992D-07	0.1113806D-01
0.9631993D+01	0.2963965D-04	0.1759120D-07	0.1116770D-01
0.9697074D+01	0.2928729D-04	0.1737508D-07	0.1119699D-01
0.9762155D+01	0.2893885D-04	0.1716154D-07	0.1122592D-01
0.9827236D+01	0.2859430D-04	0.1695053D-07	0.1125452D-01
0.9892317D+01	0.2825358D-04	0.1674205D-07	0.1128277D-01
0.9957398D+01	0.2791667D-04	0.1653604D-07	0.1131069D-01
0.1002248D+02	0.2758354D-04	0.1633250D-07	0.1133827D-01

FOR52

DAT

File: DSKB:FOR52.DAT[6452,232] Created: 09-Dec-84 17:27:00 <055> Printed: 09-Dec-84 17:32:31
QUEUE Switches: /FILE:FORT /COPIES:1 /SPACING:1 /LIMIT:270

CONCENTRATION OF THE SPRAYED SOLUTION IN THE SUMP

#	TIME	I2	I-	HOI	IO3-	H+	IO-	I3-
1	.6508103D-01	.6819839D-05	.5374871D-04	.5119192D-04	.3311030D-06	.1000000D-08	.1172053D-05	.2707823D-06
2	.1301621D+00	.5582127D-05	.5562345D-04	.5137212D-04	.7876643D-06	.1000000D-08	.5809308D-06	.2679215D-06
3	.1952431D+00	.5119425D-05	.5665989D-04	.5048114D-04	.1211987D-05	.1000000D-08	.3839081D-06	.2650972D-06
4	.2603241D+00	.4851127D-05	.5744250D-04	.4938936D-04	.1606008D-05	.1000000D-08	.2854104D-06	.2623089D-06
5	.3254052D+00	.4661268D-05	.5809266D-04	.4826376D-04	.1972427D-05	.1000000D-08	.2263228D-06	.2595561D-06
6	.3904862D+00	.4511275D-05	.5865399D-04	.4715501D-04	.2313774D-05	.1000000D-08	.1869402D-06	.2568385D-06
7	.4555672D+00	.4384656D-05	.5914749D-04	.4608131D-04	.2632303D-05	.1000000D-08	.1588177D-06	.2541557D-06
8	.5206483D+00	.4273195D-05	.5958539D-04	.4504906D-04	.2930019D-05	.1000000D-08	.1377327D-06	.2515071D-06
9	.5857293D+00	.4172321D-05	.5997580D-04	.4405987D-04	.3208658D-05	.1000000D-08	.1213395D-06	.2488924D-06
10	.6508103D+00	.4079308D-05	.6032463D-04	.4311310D-04	.3469922D-05	.1000000D-08	.1082305D-06	.2463111D-06
11	.7158914D+00	.3992399D-05	.6063645D-04	.4220720D-04	.3715100D-05	.1000000D-08	.9750998D-07	.2437629D-06
12	.7809724D+00	.3910414D-05	.6091492D-04	.4134018D-04	.3945480D-05	.1000000D-08	.8858091D-07	.2412473D-06
13	.8460534D+00	.3832548D-05	.6116313D-04	.4050987D-04	.4162195D-05	.1000000D-08	.8102987D-07	.2387640D-06
14	.9111344D+00	.3750209D-05	.6138372D-04	.3971406D-04	.4366263D-05	.1000000D-08	.7456157D-07	.2363125D-06
15	.9762155D+00	.3686916D-05	.6157897D-04	.3895076D-04	.4558628D-05	.1000000D-08	.6895948D-07	.2338925D-06
16	.1041297D+01	.3618366D-05	.6175087D-04	.3821791D-04	.4740075D-05	.1000000D-08	.6406118D-07	.2315035D-06
17	.1106378D+01	.3552264D-05	.6190119D-04	.3751369D-04	.4911379D-05	.1000000D-08	.5974248D-07	.2291451D-06
18	.1171459D+01	.3488411D-05	.6203153D-04	.3683630D-04	.5073228D-05	.1000000D-08	.5590679D-07	.2268170D-06
19	.1236540D+01	.3426591D-05	.6214332D-04	.3618422D-04	.5226228D-05	.1000000D-08	.5247785D-07	.[illegible]681700D-06
20	.1301621D+01	.3366698D-05	.6223784D-04	.3555585D-04	.5370969D-05	.1000000D-08	.4939465D-07	.2222502D-06
21	.1366702D+01	.3308557D-05	.623[illegible]627D-04	.3494988D-04	.5507959D-05	.1000000D-08	.4660781D-07	.2200106D-06
22	.1431783D+01	.3252092D-05	.6237965D-04	.3436500D-04	.5637674D-05	.1000000D-08	.4407691D-07	.2177999D-06
23	.1496864D+01	.3197189D-05	.6242900D-04	.3380000D-04	.5760571D-05	.1000000D-08	.4176858D-07	.2156175D-06
24	.1561945D+01	.3143762D-05	.6246518D-04	.3325382D-04	.5877033D-05	.1000000D-08	.3965500D-07	.2134632D-06
25	.1627026D+01	.3091735D-05	.6248905D-04	.3272537D-04	.5987461D-05	.1000000D-08	.3771279D-07	.2113366D-06
26	.1692107D+01	.3041043D-05	.6250135D-04	.3221374D-04	.6092184D-05	.1000000D-08	.3592219D-07	.2092373D-06
27	.1757188D+01	.2991623D-05	.6250275D-04	.3171807D-04	.6191517D-05	.1000000D-08	.3426636D-07	.2071650D-06
28	.1822269D+01	.2943412D-05	.6249395D-04	.3123751D-04	.6285764D-05	.1000000D-08	.3273085D-07	.2051193D-06
29	.1887350D+01	.2896367D-05	.6247551D-04	.3077131D-04	.6375200D-05	.1000000D-08	.3130322D-07	.2030999D-06
30	.1952431D+01	.2850435D-05	.6244800D-04	.3031876D-04	.6460073D-05	.1000000D-08	.2997268D-07	.2011064D-06
31	.2017512D+01	.2805588D-05	.6241190D-04	.2987922D-04	.6540617D-05	.1000000D-08	.2872984D-07	.1991386D-06
32	.2082593D+01	.2761734D-05	.6236779D-04	.2945204D-04	.6617074D-05	.1000000D-08	.2756648D-07	.1971960D-06
33	.2147674D+01	.2718871D-05	.6231609D-04	.2903662D-04	.6689654D-05	.1000000D-08	.2647537D-07	.1952784D-06
34	.2212755D+01	.2677003D-05	.6225713D-04	.2863245D-04	.6758522D-05	.1000000D-08	.2545013D-07	.1933855D-06

35	.2277836D+01	.2636006D-05	.6219183D-04	.2823904D-04	.6823885D-05	.1000000D-08	.2448513D-07	.1915168D-06
36	.2342917D+01	.2595901D-05	.6211932D-04	.2785587D-04	.6885910D-05	.1000000D-08	.2357533D-07	.1896721D-06
37	.2407998D+01	.2556666D-05	.6204112D-04	.2748251D-04	.6944749D-05	.1000000D-08	.2271627D-07	.1878510D-06
38	.2473079D+01	.2518239D-05	.6195719D-04	.2711855D-04	.7000556D-05	.1000000D-08	.2190393D-07	.1860534D-06
39	.2538160D+01	.2480610D-05	.6186783D-04	.2676358D-04	.7053479D-05	.1000000D-08	.2113473D-07	.1842787D-06
40	.2603241D+01	.2443790D-05	.6177327D-04	.2641723D-04	.7103633D-05	.1000000D-08	.2040542D-07	.1825268D-06
41	.2668322D+01	.2407690D-05	.6167388D-04	.2607917D-04	.7151158D-05	.1000000D-08	.1971309D-07	.1807974D-06
42	.2733403D+01	.2372303D-05	.6156988D-04	.2574906D-04	.7196172D-05	.1000000D-08	.1905509D-07	.1790901D-06
43	.2798484D+01	.2337132D-05	.6146150D-04	.2542656D-04	.7238783D-05	.1000000D-08	.1842903D-07	.1774047D-06
44	.2863565D+01	.2303650D-05	.6134857D-04	.2511140D-04	.7279095D-05	.1000000D-08	.1783273D-07	.1757408D-06
45	.2928646D+01	.2270334D-05	.6123250D-04	.2480330D-04	.7317206D-05	.1000000D-08	.1726420D-07	.1740982D-06
46	.2993727D+01	.2237671D-05	.6111228D-04	.2450199D-04	.7353209D-05	.1000000D-08	.1672163D-07	.1724766D-06
47	.3058808D+01	.2205659D-05	.6098850D-04	.2420723D-04	.7387188D-05	.1000000D-08	.1620336D-07	.1708757D-06
48	.3123889D+01	.2174171D-05	.6086147D-04	.2391883D-04	.7419246D-05	.1000000D-08	.1570787D-07	.1692952D-06
49	.3188971D+01	.2143343D-05	.6073119D-04	.2363645D-04	.7449445D-05	.1000000D-08	.1523377D-07	.1677348D-06
50	.3254052D+01	.2113050D-05	.6059795D-04	.2335997D-04	.7477879D-05	.1000000D-08	.1477977D-07	.1661944D-06
51	.3319133D+01	.2083363D-05	.6046181D-04	.2308913D-04	.7504603D-05	.1000000D-08	.1434468D-07	.1646736D-06
52	.3384214D+01	.2054171D-05	.6032302D-04	.2282380D-04	.7529694D-05	.1000000D-08	.1392741D-07	.1631721D-06
53	.3449295D+01	.2025559D-05	.6018162D-04	.2256372D-04	.7553212D-05	.1000000D-08	.1352695D-07	.1616897D-06
54	.3514376D+01	.1997453D-05	.6003780D-04	.2230877D-04	.7575223D-05	.1000000D-08	.1314237D-07	.1602262D-06
55	.3579457D+01	.1969818D-05	.5989173D-04	.2205879D-04	.7595785D-05	.1000000D-08	.1277279D-07	.1587812D-06
56	.3644538D+01	.1942679D-05	.5974349D-04	.2181360D-04	.7614961D-05	.1000000D-08	.1241741D-07	.1573546D-06
57	.3709619D+01	.1916038D-05	.5959317D-04	.2157302D-04	.7632805D-05	.1000000D-08	.1207549D-07	.1559461D-06
58	.3774700D+01	.1889872D-05	.5944090D-04	.2133693D-04	.7649355D-05	.1000000D-08	.1174631D-07	.1545553D-06
59	.3839781D+01	.1864157D-05	.5928679D-04	.2110521D-04	.7664668D-05	.1000000D-08	.1142924D-07	.1531822D-06
60	.3904862D+01	.1838884D-05	.5913095D-04	.2087771D-04	.7678790D-05	.1000000D-08	.1112366D-07	.1518264D-06
61	.3969943D+01	.1814082D-05	.5897348D-04	.2065430D-04	.7691768D-05	.1000000D-08	.1082901D-07	.1504878D-06
62	.4035024D+01	.1789622D-05	.5881447D-04	.2043488D-04	.7703644D-05	.1000000D-08	.1054476D-07	.1491660D-06
63	.4100105D+01	.1765617D-05	.5865401D-04	.2021931D-04	.7714458D-05	.1000000D-08	.1027040D-07	.1478608D-06
64	.4165186D+01	.1742018D-05	.5849217D-04	.2000748D-04	.7724251D-05	.1000000D-08	.1000547D-07	.1465721D-06
65	.4230267D+01	.1718821D-05	.5832903D-04	.1979929D-04	.7733055D-05	.1000000D-08	.9749532D-08	.1452996D-06
66	.4295348D+01	.1696020D-05	.5816468D-04	.1959463D-04	.7740917D-05	.1000000D-08	.9502178D-08	.1440431D-06
67	.4360429D+01	.1673613D-05	.5799916D-04	.1939341D-04	.7747858D-05	.1000000D-08	.9263018D-08	.1428023D-06
68	.4425510D+01	.1651521D-05	.5783264D-04	.1919558D-04	.7753919D-05	.1000000D-08	.9031689D-08	.1415770D-06
69	.4490591D+01	.1629812D-05	.5766509D-04	.1900099D-04	.7759132D-05	.1000000D-08	.8807847D-08	.1403671D-06
70	.4555672D+01	.1608471D-05	.5749660D-04	.1880956D-04	.7763520D-05	.1000000D-08	.8591168D-08	.1391723D-06
71	.4620753D+01	.1587509D-05	.5732720D-04	.1862119D-04	.7767125D-05	.1000000D-08	.8381347D-08	.1379924D-06
72	.4685834D+01	.1566805D-05	.5715708D-04	.1843590D-04	.7769967D-05	.1000000D-08	.8178096D-08	.1368272D-06
73	.4750915D+01	.1546482D-05	.5698616D-04	.1825340D-04	.7772073D-05	.1000000D-08	.7981141D-08	.1356765D-06
74	.4815996D+01	.1526520D-05	.5681449D-04	.1807391D-04	.7773466D-05	.1000000D-08	.7790225D-08	.1345401D-06
75	.4881077D+01	.1506790D-05	.5664227D-04	.1789719D-04	.7774175D-05	.1000000D-08	.7605103D-08	.1334178D-06
76	.4946158D+01	.1487433D-05	.5646940D-04	.1772313D-04	.7774230D-05	.1000000D-08	.7425544D-08	.1323094D-06
77	.5011239D+01	.1468353D-05	.5629601D-04	.1755175D-04	.7773645D-05	.1000000D-08	.7251328D-08	.1312147D-06
78	.5076320D+01	.1449584D-05	.5612212D-04	.1738294D-04	.7772445D-05	.1000000D-08	.7082246D-08	.1301335D-06
79	.5141402D+01	.1431142D-05	.5594773D-04	.1721663D-04	.7770649D-05	.1000000D-08	.6918101D-08	.1290657D-06
80	.5206483D+01	.1412925D-05	.5577300D-04	.1705284D-04	.7768282D-05	.1000000D-08	.6758705D-08	.1280110D-06
81	.5271564D+01	.1395057D-05	.5559783D-04	.1689139D-04	.7765360D-05	.1000000D-08	.6603878D-08	.1269693D-06
82	.5336645D+01	.1377389D-05	.5542241D-04	.1673236D-04	.7761907D-05	.1000000D-08	.6453452D-08	.1259404D-06
83	.5401726D+01	.1360065D-05	.5524663D-04	.1657557D-04	.7757935D-05	.1000000D-08	.6307264D-08	.1249241D-06
84	.5466807D+01	.1342936D-05	.5507067D-04	.1642108D-04	.7753469D-05	.1000000D-08	.6165159D-08	.1239202D-06
85	.5531888D+01	.1326113D-05	.5489443D-04	.1626873D-04	.7748520D-05	.1000000D-08	.6026991D-08	.1229286D-06
86	.5596969D+01	.1309528D-05	.5471807D-04	.1611858D-04	.7743109D-05	.1000000D-08	.5892619D-08	.1219491D-06
87	.5662050D+01	.1293203D-05	.5454153D-04	.1597050D-04	.7737249D-05	.1000000D-08	.5761911D-08	.1209815D-06
88	.5727131D+01	.1277118D-05	.5436488D-04	.1582448D-04	.7730956D-05	.1000000D-08	.5634737D-08	.1200257D-06
89	.5792212D+01	.1261267D-05	.5418815D-04	.1568047D-04	.7724250D-05	.1000000D-08	.5510975D-08	.1190815D-06
90	.5857293D+01	.1245680D-05	.5401134D-04	.1553841D-04	.7717137D-05	.1000000D-08	.5390511D-08	.1181487D-06
91	.5922374D+01	.1230288D-05	.5383454D-04	.1539831D-04	.7709637D-05	.1000000D-08	.5273230D-08	.1172272D-06
92	.5987455D+01	.1215184D-05	.5365767D-04	.1526004D-04	.7701758D-05	.1000000D-08	.5159028D-08	.1163168D-06
93	.6052536D+01	.1200244D-05	.5348090D-04	.1512368D-04	.7693518D-05	.1000000D-08	.5047802D-08	.1154174D-06
94	.6117617D+01	.1185530D-05	.5330416D-04	.1498911D-04	.7684926D-05	.1000000D-08	.4939453D-08	.1145288D-06
95	.6182698D+01	.1171066D-05	.5312747D-04	.1485629D-04	.7675999D-05	.1000000D-08	.4833889D-08	.1136508D-06
96	.6247779D+01	.1156775D-05	.5295092D-04	.1472525D-04	.7666745D-05	.1000000D-08	.4731019D-08	.1127834D-06
97	.6312860D+01	.1142738D-05	.5277444D-04	.1459586D-04	.7657174D-05	.1000000D-08	.4630757D-08	.1119263D-06
98	.6377941D+01	.1128879D-05	.5259813D-04	.1446818D-04	.7647300D-05	.1000000D-08	.4533021D-08	.1110795D-06
99	.6443022D+01	.1115195D-05	.5242201D-04	.1434215D-04	.7637134D-05	.1000000D-08	.4437731D-08	.1102427D-06
100	.6508103D+01	.1101761D-05	.5224602D-04	.1421768D-04	.7626683D-05	.1000000D-08	.4344812D-08	.1094159D-06
101	.6573184D+01	.1088490D-05	.5207026D-04	.1409401D-04	.7615955D-05	.1000000D-08	.4254189D-08	.1085989D-06
102	.6638265D+01	.1075398D-05	.5189475D-04	.1397351D-04	.7604973D-05	.1000000D-08	.4165792D-08	.1077916D-06
103	.6703346D+01	.1062518D-05	.5171945D-04	.1385370D-04	.7593733D-05	.1000000D-08	.4079555D-08	.1069938D-06
104	.6768427D+01	.1049829D-05	.5154439D-04	.1373537D-04	.7582247D-05	.1000000D-08	.3995411D-08	.1062054D-06
105	.6833506D+01	.1037287D-05	.5136964D-04	.1361853D-04	.7570525D-05	.1000000D-08	.3913299D-08	.1054263D-06
106	.6898589D+01	.1024933D-05	.5119518D-04	.1350312D-04	.7558577D-05	.1000000D-08	.3833158D-08	.1046563D-06
107	.6963670D+01	.1012793D-05	.5102097D-04	.1338908D-04	.7546467D-05	.1000000D-08	.3754930D-08	.1038953D-06
108	.7028751D+01	.1000785D-05	.5084713D-04	.1327646D-04	.7534027D-05	.1000000D-08	.3678560D-08	.1031432D-06
109	.7093832D+01	.9889332D-06	.5067364D-04	.1316522D-04	.7521444D-05	.1000000D-08	.3603992D-08	.1023999D-06
110	.7158914D+01	.9772912D-06	.5050045D-04	.1305526D-04	.7508664D-05	.1000000D-08	.3531177D-08	.1016652D-06
111	.7223995D+01	.9658023D-06	.5032763D-04	.1294664D-04	.7495654D-05	.1000000D-08	.3460063D-08	.1009391D-06
112	.7289076D+01	.9544450D-06	.5015521D-04	.1283932D-04	.7482544D-05	.1000000D-08	.3390603D-08	.1002214D-06
113	.7354157D+01	.9432469D-06	.4998318D-04	.1273328D-04	.7469220D-05	.1000000D-08	.3322750D-08	.9951194D-07
114	.7419238D+01	.9322595D-06	.4981149D-04	.1262842D-04	.7455725D-05	.1000000D-08	.3256459D-08	.9881069D-07
115	.7484319D+01	.9213837D-06	.4964025D-04	.1252484D-04	.7442065D-05	.1000000D-08	.3191687D-08	.9811749D-07
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117	.7614481D+01	.9000500D-06	.4929908D-04	.1232128D-04	.7414298D-05	.1000000D-08	.3066533D-08	.9675485D-07
118	.7679562D+01	.8896563D-06	.4912909D-04	.1222121D-04	.7400193D-05	.1000000D-08	.3006071D-08	.9608519D-07
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126	.8200210D+01	.8111563D-06	.4778648D-04	.1146066D-04	.7282841D-05	.1000000D-08	.2568414D-08	.9099390D-07

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129	.8395453D+01	.7838775D-06	.4729119D-04	.1119252D-04	.7237085D-05	.1000000D-08	.2423275D-08	.8920003D-07
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137	.8916101D+01	.7162693D-06	.4599435D-04	.1051883D-04	.7111626D-05	.1000000D-08	.2079235D-08	.8469835D-07
138	.8981182D+01	.7083153D-06	.4583476D-04	.1043861D-04	.7095656D-05	.1000000D-08	.2040206D-08	.8416294D-07
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141	.9176425D+01	.6850434D-06	.4535951D-04	.1020295D-04	.7047443D-05	.1000000D-08	.1927920D-08	.8259115D-07
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153	.9957398D+01	.6006656D-06	.4351169D-04	.9330051D-05	.6851377D-05	.1000000D-08	.1542343D-08	.7678515D-07
154	.1002248D+02	.5942123D-06	.4336163D-04	.9261990D-05	.6834892D-05	.1000000D-08	.1514261D-08	.7633366D-07

Appendix F

LIST OF SYMBOLS

A	Input starting time for all numerical models
a_n	nth root of $a_n \cot(a_n) - (N_{sh}-1) = 0$
B	Input stopping time for KINETIC and DROP models
BWR	Boiling Water Reactor
C	Concentration of a species
C_g	Concentration of a species in the gas phase
C_{gi}	Concentration of a species in the gas phase at the interface
C_l	Concentration of a species in the liquid phase
C_{li}	Concentration of a species in the liquid phase at the interface
cc	Cubic centimeter
CDIAM	Containment diameter in the SPRAY and WALL-SPRAY models, meters
CHL	Containment of hydrogen ions, H^+, in the liquid for the DROP and KINETIC models, moles/liter
CHOIL	Concentration of hypoiodous acid, HOI, in the liquid for the KINETIC and DROP models, moles/liter
CHOISP	Concentration of hypoiodous acid, HOI, in the spray solution for the SPRAY and WALL-SPRAY models, moles/liter
CHSP	Concentration of hydrogen ions H^+ in the spray solution for the SPRAY and WALL-SPRAY models, moles/liter
CIL	Concentration of Iodide, I^-, in the liquid for the KINETIC and DROP models, moles/liter
CISP	Concentration of Iodide ion, I^-, in the spray solution for the SPRAY and WALL-SPRAY models, moles/liter.
CI03L	Concentration of Iodate ion, IO_3^- in the liquid for the KINETIC and DROP models, moles/liter.
CI03SP	Concentration of Iodate ion, IO_3^-, in the spray solution for the SPRAY and WALL-SPRAY models, moles/liter.
CI2L	Concentration of molecular iodine, I_2, in the liquid for the KINETIC and DROP models, moles/liter.
CI2SP	Concentration of molecular Iodine, I_2, in the spray solution for the SPRAY and WALL-SPRAY models, moles/liter.
cm	Centimeters

COIL	Concentration of Hypo-iodate ion, OI^-, in the liquid for the KINETIC and DROP models, moles/liter.
COISP	Concentration of Hypo-Iodate ion, OI^-, in the spray solution for the SPRAY and WALL-SPRAY models, moles/liter.
cot	Cotangent
cP	CentiPoise
CPU	Central Processor Unit
CSE	Containment Systems Experiments
d	Drop diameter
D_g	Diffusion coefficient for the gas
D_l	Diffusion coefficient for the liquid
DENGAS	Density of air, gms/cc
DENLIQ	Density of water, gms/cc
DIAM	Drop diameter, cm
DURTM	Duration of spray, min
E	Spray removal efficiency
exp	exponential
EXPTM	Exposure time, seconds
F	Flow rate
FLRAT	Flow rate, liter/min
g	Acceleration of gravity
h	Drop fall height
H^+	Hydrogen ion
HEIGHT	Drop fall height, m
HMAX	Maximum step size for the RKF numerical integration routine
HMIN	Minimum step size for the RKF numerical integration routine
HOI	Hypoiodous Acid
IN	Number of equations to integrate. 4 for buffered solution; 5 for unbuffered solution
I^-	Iodide
I_2	Molecular Iodine
I_3^-	Tri-Iodide
IO_3^-	Iodate ion
K	Kelvin
k_i	Reaction rate constant for equation i. ($i < 0$: reverse reaction, $i > 0$: forward reaction)

K_i	Equilibrium constant for equation i.
k_g	Gas side mass transfer coefficient
K_{gov}	Overall gas side mass transfer coefficient
k_l	Liquid side mass transfer coefficient
K_{lov}	Overall liquid side mass transfer coefficient
$k_{l,av}$	Average mass transfer cofficient for a falling liquid film
Ln	Natural logarithm
Log	Base 10 logarithm
$\underline{M}$	Molarity, moles/liter
M_a	Molecular weight of species a
M_b	Molecular weight of species b
M_r	Mass transfer rate
N_A	Mass transfer flux to the drop
$N_{A,w}$	Mass transfer flux to the liquid on walls
N_D	"Best Number"
N_{re}	Reynolds number
OI^-	Hypo-Iodate ion
OH^-	Hydroxide ion
p	Pressure
P	Partition coefficient
PRESS	Pressure, atm
PWR	Pressurized water reactor
r	Distance from the outer radius of the drop
R	Reaction rate
s	Seconds
sec	Seconds
Sc	Schmidt number
t	Time
t^*	Contact time for each element in a drop
t_e	Exposure time of a drop
$t_{1/2}$	Half life
T	Temperature
TEMPG	Temperature of the gas, K
TEMPL	Temperature of the liquid, K
TOLER	Relative error control for RKF routine

TRMVEL	Terminal velocity of a drop, cm/sec
u	Velocity < vector >
v	Velocity
v_g	Terminal settling velocity
V	Containment volume
VISGAS	Viscosity of the gas phase, cP
VISLIQ	Viscosity of the liquid phase, cP
WFRAC	Fraction of spray flow rate which flows down the wall
WHT	Wall height, meters
WOLD(1)	Concentration of I_2 in RKF routine, moles/liter
WOLD(2)	Concentration of I^- in RKF routine, moles/liter
WOLD(3)	Concentration of HOI in RKF routine, moles/liter
WOLD(4)	Concentration of IO_3^- in RKF routine, moles/liter
WOLD(5)	Concentration of H^+ in RKF routine, moles/liter
WOLD(6)	Concentration of OI^- in RKF routine, moles/liter
WOLD(7)	Concentration of I_3^- in RKF routine, moles/liter
λ	Removal rate constant
Φ	$4 D_e t_e/d^2$
σ	Thickness of water on the walls
Ω	Collision integral
ρ	Density
μ	Viscosity
∇	Nable operator
Δ^2	Laplacian operator

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13. ABSTRACT (200 words or less)
A new model has been developed for predicting the rate at which gaseous molecular iodine is absorbed by water sprays. The model is a quasi-steady state mass transfer model that includes the iodine hydrolysis reactions. The parameters of the model are spray drop size, initial concentration of the gas and liquid phases, temperature, pressure, buffered or unbuffered spray solution, spray flow rate, containment diameter and drop fall height. The results of the model were studied under many values of these parameters. Plots of concentration of iodine species in the drop versus time have been produced by varying the initial gas phase concentration of molecular iodine over the range of 1×10^{-5} moles/liter to 1×10^{-10} moles/liter, a buffered pH of 7 or 9, and a drop size of 1000 microns.

Results from the model are compared to results available from the Containment Systems Experiments at Pacific Northwest Laboratory. The difference between the model predictions and the experimental data ranges from -120% to 68% with the closest agreement 7.7%. The new spray model is also compared to previously existing spray models. At high concentrations of gaseous molecular iodine, the new spray model is considered to be less accurate than the previous models. At low concentrations, the new model predicts results that are closer to the experimental data. Inclusion of the iodine hydrolysis reactions is shown to be important for determining the removal of molecular iodine from gas phase by water sprays for most conditions.

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