EPA/600/A-92/235

MULTIZONAL MASS BALANCE MODELING OF BENZENE DISPERSION IN A PRIVATE RESIDENCE

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ABSTRACT

A residence in Roxboro, NC, was found to have its well-water supply contaminated with benzene ($\approx$ 300 μg/l) and other organic compounds. The residents of the house do not currently drink the water, but they use it for daily showers. A study was designed to monitor and model short-term benzene dispersion within the house during and after a shower.

A multizonal mass balance model, CONTAM88, was used to predict interzonal air flow rates and benzene concentration distributions within the house. The idealization of the building was created using NBSAVIS, a preprocessor to CONTAM88. Simulation results showed that the highest concentration occurred in the shower stall. During the shower, the master bathroom concentration was less than half the shower-stall concentration. Benzene concentrations in the master bedroom and other rooms were lower. Simulated benzene concentration distributions showed that benzene from the shower rapidly dispersed in the house, and reached equilibrium in all the rooms in less than 30 minutes after the shower. These results were supported by SF6 experimental data.

Benzene samples were collected using glass, gas-tight syringes in the shower stall and at various locations in the house. The average benzene concentration after a 20-minute shower was 978 $\mu g/m^3$ in the shower stall, 263 $\mu g/m^3$ in the master bathroom, and 70 $\mu g/m^3$ in the master bedroom. Simulated and average measured benzene concentrations yielded a similar behavioral trend. It was concluded that multizonal mass balance models may be useful in designing field study monitoring strategies.

Keyword index: Indoor air, multizonal models, mass balance models, contaminant dispersion, benzene, shower, SF6.

INTRODUCTION

Benzene has the largest production volume of any chemical that has been causally linked to cancer in humans.[1] It is a pollutant that is spread in the environment from sources such as tobacco smoke, automobile refueling, and industrial waste.[2,3,4] Residential use of benzene-contaminated water may result in significant inhalation, ingestion, and dermal exposures.[5]

Previous investigations have shown that trichloroethylene (TCE) contaminated water supply may constitute a significant point source of human exposure for the bather, and a dispersed source for other inhabitants in the home. For highly volatile chemicals, inhalation exposures have the potential to be equal or greater than those associated with direct ingestion of water.[6,7] For households using tap water contaminated with TCE, inhalation exposures in showers could be as large as or larger than a conservative estimate of ingestion exposure. The assumption that a 70-kg adult consumes 2 liters (l) per day of tap water was considered a conservative estimate of ingestion exposure.[8]

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In 1985, a residence in Roxboro, NC, was identified as using ground water contaminated with benzene, xylene, and other organic compounds. The benzene contamination has been characterized by measurements of 7 μg/l, 32 μg/l, and 445 μg/l in 1986, 1989, and 1990, respectively. The homeowners have continued to reside in the house and use the water for all their normal purposes except drinking and cooking. In 1991, the U.S. Environmental Protection Agency (EPA) conducted a series of tests to assess shower-related exposures that occur throughout the house during and after a single 20-minute shower, to determine the relationship between various monitoring techniques and to assess the usefulness of multizonal mass balance models during experimental study designs.

STUDY OBJECTIVES

The objectives of this study are to (1) investigate the possibility of using multizonal mass balance models to predict locations where benzene concentrations are significantly different from background concentrations in order to optimize sampling times and locations during a field study design, and (2) test the model performance in a well-defined microenvironment.

THE MULTIZONAL MASS BALANCE MODEL, CONTAM88

The multizonal mass balance model used in this investigation is the National Institute of Standards and Technology (NIST) model, NBSAVIS/CONTAM88[9] developed for EPA, to simulate transient contaminant concentration distribution in buildings. The model is based on the element-assembly approach, which assumes that a building can be represented as a combination of well-mixed zones linked by flow and kinetic elements (contaminant mass transport and decay). CONTAM88 solves a set of mass balance and flow equations. The mathematical formulation of the contaminant concentration is:

$$[W]\vec{C} + [M]\frac{d\vec{C}}{dt} = \vec{G}$$

where:
- $\vec{C}$ = vector containing the discrete concentration values
- $[W]$ = system mass transport matrix containing flow rate data
- $[M]$ = system matrix containing mass (volume) data
- $\vec{G}$ = system generation vector containing kinetics data.

NBSAVIS is a preprocessor to CONTAM88 that allows the idealization of the building through the generation of a file that describes the building configuration, including indoor and outdoor contaminant sources. Data input to NBSAVIS are controlled by a series of screen-fill subroutines, which allow the user to specify interior and exterior wall types, interior and exterior doors, windows, open passageways, filters and fans, room descriptions, and HVAC system descriptions.

RESIDENCE DESCRIPTION AND IDEALIZATION

The private residence, which is located in a rural area in Roxboro, NC, is a single-story house. The house has three bedrooms, a bathroom, a family room, a laundry room, and an open area that consists of a living room, kitchen, and dining room (Figure 1). The master bedroom area includes a bathroom with a separate shower. The house also has a full basement, an attic, and a carport. The residents of the house get their water from a nearby well, located south of the residence.

The NBSAVIS preprocessor was used to build the idealization of the house. The parameters of the house that were measured to run NBSAVIS are as follows:

- Physical dimensions (including all windows, doors, and other openings),
- HVAC system output, including locations of all vents and the associated air flow rates,
- Contaminant source information (name, molecular weight, emission rate),
- Source locations (outside or inside, particular rooms of the house), and
- Local meteorological conditions (temperature, wind speed, and wind direction).

RESULTS AND DISCUSSION

Air flow rates from all the vents of the HVAC system were measured using an Omega HH-30 vane anemometer; the HVAC return flow rate (Table 1) was measured using a Shortridge Instruments Flow Hood. Constant meteorological conditions were assumed, because the duration of the simulations did not exceed 4 hours. The estimated local meteorological conditions were: 2 m/s wind speed, 220° wind direction, and 25 °C temperature.

In the first stage of the study, a 15-minute shower was simulated--with water temperature of approximately 40 °C, at a flow rate of 10 l/minute. The contaminant, benzene, was modeled as a point source located in the shower stall. The most recent benzene-in-water concentration (445 μg/l measured in the house in 1990) and a 61% transfer efficiency of TCE from shower water-to-air (from McKone and Knezovich[8]) were used to estimate the benzene emission rate--45 μg/s. Also, sulfur hexafluoride (SF6) was released in the shower for 15 minutes and its dispersion was monitored throughout the residence. Syringe samplers were placed in all rooms of the house (one sampler per room, in a location not exposed to direct air flow from the vents) to monitor concentration gradients.

Each room in the house was considered as one zone, except the master bathroom which was considered as two zones because it has a separate shower stall. During the entire testing period, the HVAC system was running (only fan on). The ceiling fans were also running at their lowest speed to allow constant contaminant mixing without disturbing interzonal air flows. Using the above conditions, benzene dispersion throughout the house during and after the shower was simulated.

Simulation results for the first stage of this study showed that the highest benzene concentrations occurred in the shower and master bathroom, then in decreasing concentrations, in the master bedroom and hallway. The living room, dining room, kitchen, and family room had lower concentrations. These results were supported by the SF6 experimental data (Figure 2). Modeled benzene concentration distributions showed that benzene rapidly dispersed in the house, and all rooms in the house reached equilibrium within 30 minutes after the shower (Figures 3a and 3b). Therefore, a total sampling time of about 50 minutes may be chosen. After that time, simulated concentrations of about 50 $\mu g/m^3$ were found in the house.

In the second stage of the study, the living room, dining room, kitchen, and family room were considered as one well-mixed zone. Furthermore, the total simulation time was 50 minutes. The shower was run for 20 minutes with the bathroom door closed. After the shower, the shower-stall door was open and the bathroom door was kept closed for 5 minutes to allow for the individual to dry off and get dressed. After that time, the shower-stall and bathroom doors were opened. The average measured shower water flow rate was about 6.3 l/min, and the average waterborne benzene concentration from the pre-shower head samples was 292 μg/l. Waterborne benzene concentrations from the pre-shower head samples and the drain-level samples were measured and used to calculated the water-to-air transfer efficiency. The average calculated benzene transfer efficiency was 88% yielding a benzene emission rate of 27.5 μg/s. Using the above conditions, benzene dispersion throughout the house during and after the shower was simulated. Simulation results of benzene dispersion showed a benzene concentration of 625 $\mu g/m^3$ in the shower stall after a 20-minute shower, 278 $\mu g/m^3$ in the master bathroom, and 148 $\mu g/m^3$ in the master bedroom. The rest of the rooms in the house had concentrations of less than 40 $\mu g/m^3$.

Benzene concentration levels were measured during a 3-day, 3-shower period (i.e., 1 shower each day).[10] Glass, gas-tight syringe samplers were placed in the shower stall, bathroom, master bedroom, and living room. The total sampling time was 120 minutes. After 20 minutes, the shower-stall concentration reached an average value of 978 $\mu g/m^3$ (standard deviation, SD, equal to 514 $\mu g/m^3$), the master bathroom concentration reached 263 $\mu g/m^3$ (SD = 64 $\mu g/m^3$), the master bedroom concentration reached 70 $\mu g/m^3$ (SD = 14 $\mu g/m^3$), and the living room concentration reached 40 $\mu g/m^3$ (SD = 16 $\mu g/m^3$). Figures 4 and 5 show the simulated and measured benzene concentrations in the shower stall and the master bathroom, respectively.

During the shower, there was significant variability in the data, which may be due to incomplete mixing, dynamic variation in the benzene-in-water concentration, and experimental errors. The benzene concentration during the third shower was much higher than during the first two showers. This difference may be due to variability in water flow, as well as sampling inaccuracies due to incomplete mixing. Differences between simulated and measured concentrations may be due to model limitations. For instance, the assumption of a well-mixed zone may be too simplistic. Also, the assumptions and parameter estimation used in the idealization of the house may constitute a significant source of uncertainty. Overall, the model did well in predicting the zones of significantly different concentrations and the time necessary for the contaminant to reach equilibrium throughout the house.

CONCLUSIONS

In the first stage, CONTAM88 was used to plan the study design. SF6 was used to measure flow rates within the house. Modeled benzene concentrations in the shower were more than twice the master bathroom's concentration during the shower. After the shower and opening the shower door, benzene quickly dispersed in the house. Concentration equilibrium was reached within 30 minutes. This result suggests that a total sampling period of less than 50 minutes would be appropriate for this type of study. Simulation results also showed that the living room, dining room, kitchen, and family room have similar concentrations. Therefore, they were grouped into one zone. The SF6 experimental analysis yielded similar results.

In the second stage of the study, benzene concentrations were simulated and measured in the shower, master bathroom, master bedroom, and living room. The average measured shower benzene concentrations were about 40% higher than the simulated ones; the simulated master bathroom concentrations were about 6% higher than the measured ones, and the simulated master bedroom concentrations were about 100% higher than the average measured one. The simulated concentrations in the rest of the rooms were about 20% lower than the measured ones. Therefore, CONTAM88 may only be used to simulate broad trends of concentration distribution throughout the house. Using CONTAM88 for the exposure assessment suggested that a 1-hour sampling time should be appropriate for a 20-minute shower. The model also helped in deciding the rooms in which to locate the samplers, to monitor benzene concentration distribution. Simulation results will hopefully help investigators plan field studies and minimize the cost of the studies.

ACKNOWLEDGEMENTS

The authors wish to acknowledge and thank Mark Johnson and David Proffitt for the air exchange and SF6 data, used during the preliminary stage of the study. The authors also thank Larry Michael for the benzene data. This work was sponsored by the Indoor Air Research Section, U.S. Environmental Protection Agency.

DISCLAIMER

This paper has been reviewed in accordance with the U.S. Environmental Protection Agency's peer and administrative review policies and approved for presentation and publication. Mention of trade names or commercial products does not constitute endorsement or recommendation for use.

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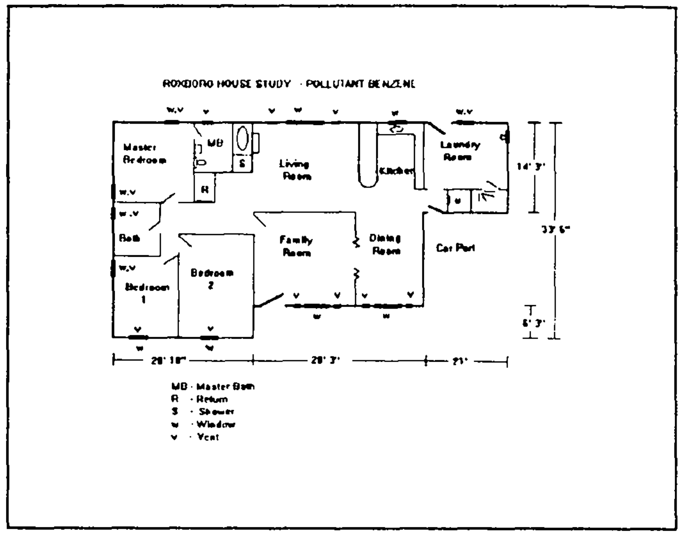

Figure 1. Roxboro house. Pollutant benzene.

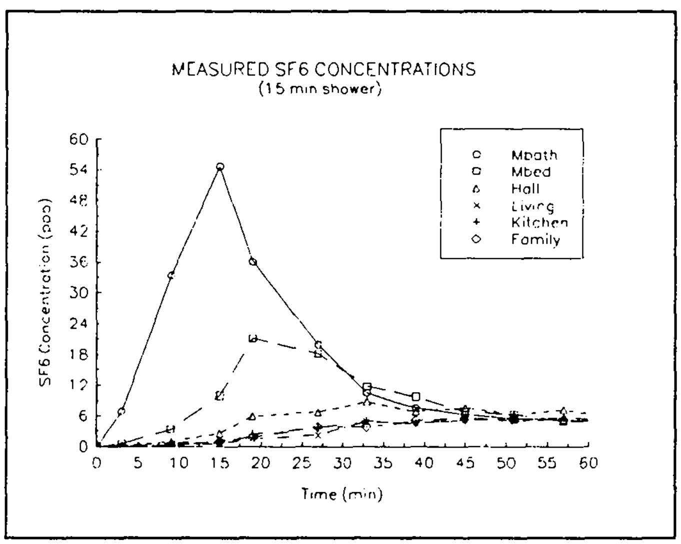

Figure 2. Measured SF6 concentration distribution within the house. During and after a 15 min shower.

Table 1. Air flow measurements from the Roxboro house.

Room-vent #	Air flow (m^3/min)
Kitchen	3.77
Laundry room	3.10
Dining room-1	2.78
Dining room-2	1.96
Family room-1	2.96
Family room-2	4.02
Bedroom 1-1	1.31
Bedroom 1-2	0.81
Bedroom 2	1.32
Bathroom	4.28
Master bedroom-1	3.02
Master bedroom-2	3.22
Master bathroom	7.14
Living room-1	3.00
Living room-2	3.29
Basement	5.92
Return	44.53

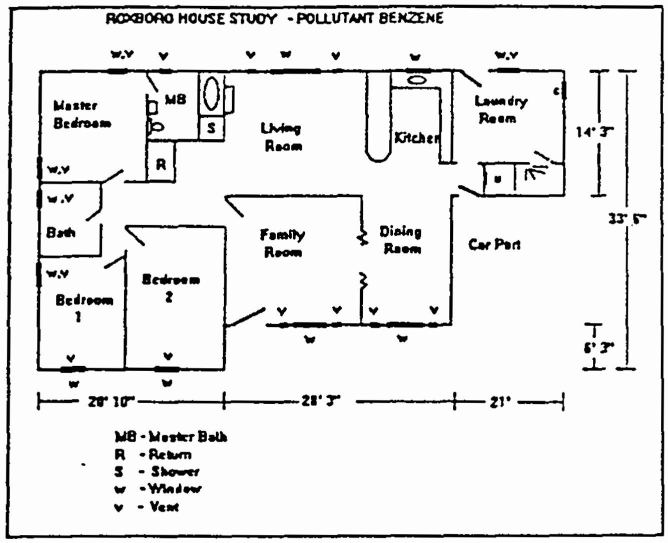

Figure 1. Schematic of the Roxboro house.

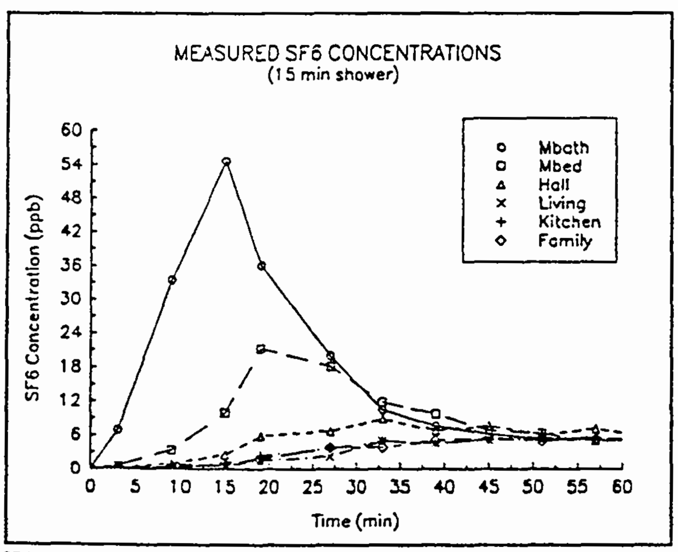

Figure 2. Measured SF6 concentration distribution within the house. During and after a 15-min. shower.

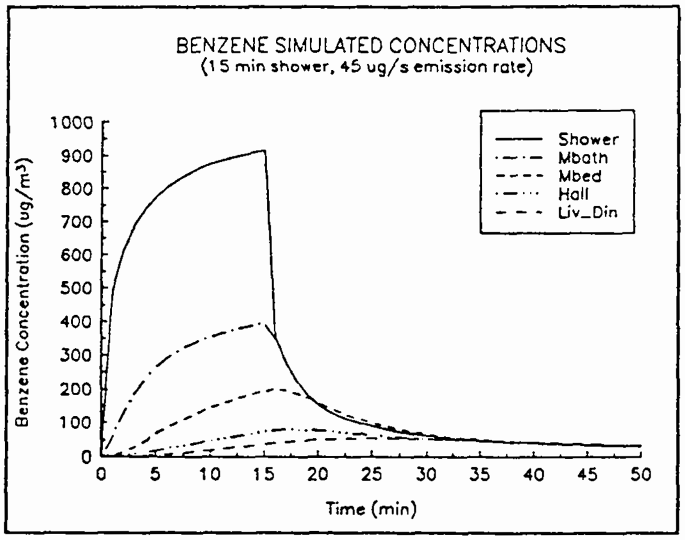

Figure 3a. Simulated benzene concentration distribution during and after a 15-min. shower, for the rooms of highest concentration levels.

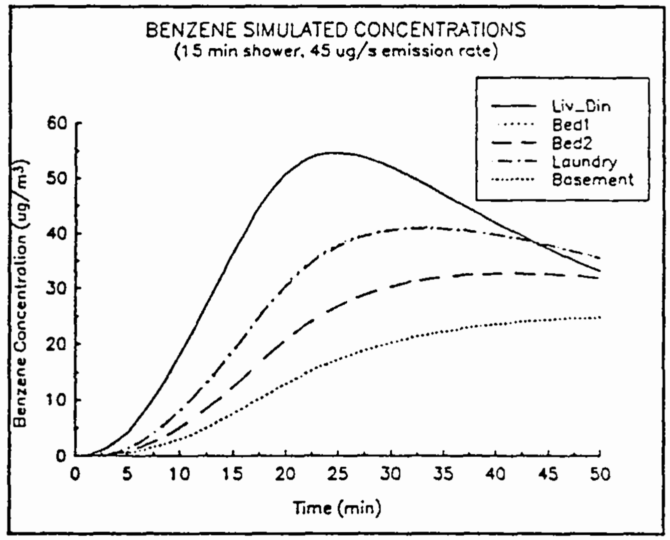

Figure 3b. Simulated benzene concentration distribution during and after a 15-min. shower, for the rest of the house.

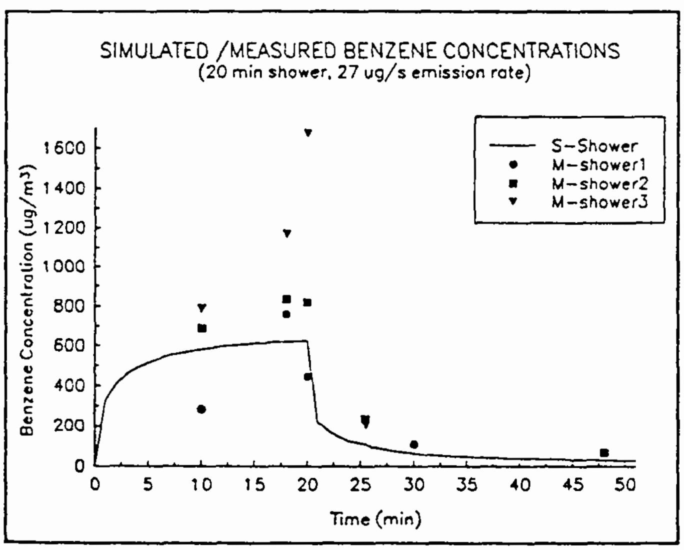

Figure 4. Simulated (S) and measured (M) benzene transient concentration in the shower stall, during a 3-day, 3-shower experiment.

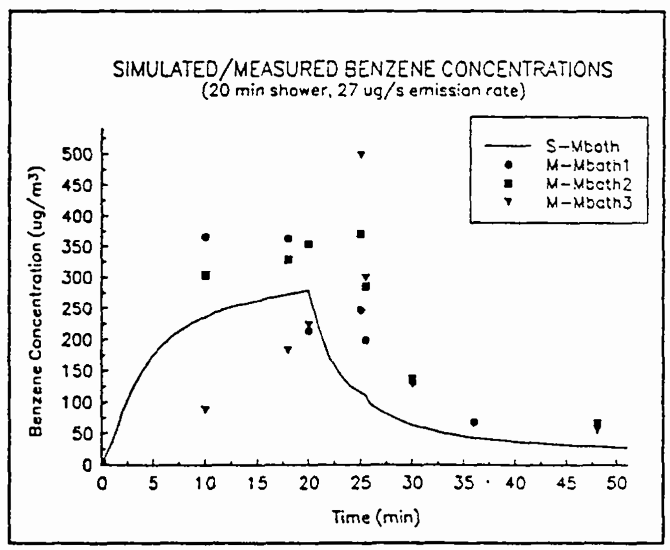

Figure 5. Simulated (S) and measured (M) benzene transient concentration in the master bathroom, during a 3-day, 3-shower experiment.

TECHNICAL REPORT DATA

1. REPORT NO. EPA/600/A-92/235	2.	3.
4. TITLE AND SUBTITLE Multizonal mass balance modeling of benzene dispersion in a private residence.		5. REPORT DATE 6. PERFORMING ORGANIZATION CODE
7. AUTHOR(S) Azzedine Lansari, CSC Andrew Lindstrom, HERB/AREAL Brian Templeman, HEMB/AREAL John S. Irwin, HEMB/AREAL		8. PERFORMING ORGANIZATION REPORT NO.
9. PERFORMING ORGANIZATION NAME AND ADDRESS Computer Science Corporation Research Triangle Park, NC 27711		10. PROGRAM ELEMENT NO. 11. CONTRACT/GRANT NO. No. 68-WO-0043
12. SPONSORING AGENCY NAME AND ADDRESS Atmospheric Research and Exposure Assessment Laboratory -- RTP Office of Research and Development U.S. Environmental Protection Agency Research Triangle Park, NC 27711		13. TYPE OF REPORT AND PERIOD COVERED 14. SPONSORING AGENCY CODE EPA/600/09

15. SUPPLEMENTARY NOTES

Proceedings of the 1992 U.S. EPA/A&WMA Symposium on Measurement of Toxic and Related Air Pollutants, Durham, NC. May 1992.

16. ABSTRACT

A residence in Roxboro, NC, was found to have its well-water supply contaminated with Benzene ($\approx 300\mu/l$) and other organic compounds. The residents of the house do not currently drink the water, but they use it for daily showers. A study was designed to monitor and model short-term benzene dispersion within the house during and after a shower.

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17. KEY WORDS AND DOCUMENT ANALYSIS

a. DESCRIPTOI	b. IDENTIFIERS/ OPEN ENDED TERMS	c. COSATI

18. DISTRIBUTION STATEMENT Release to Public	19. SECURITY CLASS (This Report) UNCLASSIFIED	21. NO. OF PAGES 8
	20. SECURITY CLASS (This Page) UNCLASSIFIED	22. PRICE