



# Project Summary

## Application of Pollution Prevention Techniques to Reduce Indoor Air Emissions from Aerosol Consumer Products

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The report gives results of research, undertaken to develop tools and methodologies to measure aerosol chemical and particle dispersion through space. Georgia Tech Research Institute researchers built an Aerosol Mass Spectral Interface (AMSI), which is interfaced with a mass spectrometer (MS), that chemically characterizes aerosol consumer products as they move through space. University of Illinois researchers developed techniques for measuring aerosol movement indoors by tracking particle size changes via particle velocity measurements using particle image velocimetry (PIV). The AMSI was designed, constructed, and optimized to transfer a focused beam of aerosol particles into a MS for chemical analysis. Experiments showed that the AMSI can quantitatively detect compositional changes as the aerosol travels through space. These data provide important information for formulating aerosol consumer products for pollution prevention strategies. The PIV system demonstrated a correlation between the material properties of the aerosol components and the spray pattern. These data were used to develop a model for predicting the major characteristics of aerosol spray patterns.

*This Project Summary was developed by the National Risk Management Research Laboratory's Air Pollution Pre-*

*vention and Control Division, Research Triangle Park, NC, to announce key findings of the research project that is fully documented in a separate report of the same title (see Project Report ordering information at back).*

### Introduction

The U.S. EPA has identified indoor air quality (IAQ) as one of the most important environmental risks to the Nation's health. In the Pollution Prevention Act of 1990, Congress declared that pollution should be prevented or reduced at the source whenever feasible. Modification of equipment, processes, and procedures; reformulations or redesign of products; substitution of raw materials; and/or improvements in use procedures may accomplish source reduction.

Aerosol consumer products potentially are amenable to pollution prevention strategies that reformulate or redesign products, substitute raw materials, and improve use procedures. For example, the tools developed under this project may provide manufacturers with data showing that products can be reformulated, thereby reducing the required amount of active ingredient. For example, if 50% more of the active ingredient is reaching the use site than is needed for efficacy, the manufacturer may be able to reduce the amount of active ingredient in the product accordingly.

A basic understanding of the behavior of aerosol consumer products can be used to develop pollution prevention strategies, which may reduce occupant exposures and guide manufacturers in the development of more efficacious products. The spray cone is the dynamic three-dimensional projection of the liquid aerosol particles ejected from the aerosol consumer product spray nozzle into the air. The length, particle sizes (and, potentially, chemical composition), and the velocity distribution are constantly changing as the aerosol disperses through space. The spray cone can be influenced by the localized air flow patterns in the space created by natural and mechanical ventilation. A basic understanding of the spray cone behavior (both the chemical composition and the particulate composition) is critical in understanding product efficacy and in devising pollution prevention strategies.

This research project was undertaken to develop tools and methodologies to measure aerosol chemical and particle dispersion through space. EPA's National Risk Management Research Laboratory sponsored a cooperative agreement with the Georgia Tech Research Institute (GTRI) and the University of Illinois (UI) to develop tools and methodologies to measure aerosol chemical composition and particle dispersion through space. These tools can be used to devise pollution prevention strategies that could reduce occupant chemical exposures and guide manufacturers in formulating more efficacious products. GTRI researchers built an Aerosol Mass Spectral Interface (AMSI), which is interfaced with a mass spectrometer (MS), that chemically characterizes aerosol consumer products as they move through space. The AMSI/MS is unique in that it measures the spatial chemical composition of the aerosol stream, rather than the more conventional technique of measuring the chemical composition of single aerosol particles. UI researchers developed techniques for measuring aerosol indoors by tracking particle size changes via particle velocity measurements using particle image velocimetry (PIV). This technique was used to develop a model to predict the major characteristics of aerosol spray patterns. Industry Partners participated in this research project to ensure that the technologies developed would be useful to industry.

### Surrogate Aerosols

The number of different aerosols is immense. A major task was development of a classification scheme representative of most of the industry, but dividing the aero-

sol products into a manageable size for meaningful data collection during the tools and methods development. Also, to maintain the scientific integrity of the project and the full cooperation of the Industry Partners, it was important that the research focus on generic products rather than any specific manufacturers' formulations. Since the purpose of the project was to develop generic tools and methods that could be used by the industry as a whole to develop pollution prevention strategies, it was important to focus on the end use of products rather than specific products.

The aerosol classification scheme developed for this project focuses on product uses because they have the greatest influence on spatial dispersion. A set of 12 surrogate aerosols, representing common formulations and uses, was developed by the Industry Partners. These fall into three categories: 1) surface wipe aerosols (aerosol products that are sprayed on a surface, then wiped off), 2) surface non-wipe aerosols (aerosol products that are sprayed on a surface and not wiped off), and 3) air sprays. These are further subdivided into the categories of liquefied hydrocarbon propellant and compressed gas propellant aerosols, since the propellant system can influence aerosol spatial dispersion and, therefore, could be important in the design of pollution prevention strategies. The surface wipe and surface non-wipe surrogates were tested both as pressurized and pump delivery systems. The surrogate aerosols were designed, prepared, and supplied by the Industry Partners.

### Chemical Composition

The AMSI can be used by industry to determine the chemical composition of aerosol particles through space. Knowing the chemical composition and the changes in the chemical composition during particle dispersion through space may guide the industry to make more efficacious products and devise pollution prevention strategies through product reformulation.

The AMSI was designed, constructed, and optimized to transfer a focused aerosol beam of particles into a MS for chemical analysis. Experiments showed that the AMSI could detect compositional changes through space, and that the AMSI was transferring aerosol particles into the MS. The data obtained in this project indicate that the AMSI/MS should be capable of quantitative analysis, but further study is required to confirm this. The AMSI/MS is unique in that it can determine chemical compositional changes as the aerosol

consumer product travels through space. Most of the current MS research of aerosols measures the chemical composition of individual aerosol particles rather than looking at the complete stream of aerosol particles.

The AMSI is essentially the momentum separator portion of a particle beam (PB) interface. The AMSI separates the aerosol particles from the propellants. This was necessary since the propellants are the major components in the aerosol spray and overloaded the MS when the aerosol was sprayed directly into the MS. The AMSI sends a focused aerosol beam of aerosol particles into the MS. The MS response with AMSI was found to be within 5% of the standard deviation from the mean peak area.

The AMSI was designed to relate chemical composition to particle size. The AMSI sends aerosol particles in a straight-line trajectory path into the MS. A gas flow was applied within the AMSI to change the particle size distribution entering the MS. When no gas flow was applied, the entire distribution of particle sizes was transferred into the MS. When a gas flow was applied, fewer of the smaller particles entered the MS, since the gas flow pushed the smaller particles off of the straight-line trajectory path.

One important finding of this research project was the detection of a contaminant in the starting materials used to make the test aerosol products. This contaminant was detectable also in the surrogate aerosols. This finding can provide important data for manufacturers in selecting starting materials to make their products.

It was found that ion/molecule reactions occur as the aerosol is ejected from the spray nozzle when components like silicone are ingredients of the aerosol consumer product. Understanding these reactions may be important in understanding product efficacy.

### Particulate Behavior

A PIV system was used to determine the particulate characteristics of the spray cone of aerosol consumer products. The PIV was used to measure particle concentrations and velocity distributions. These techniques were used in an environmental chamber to investigate the effect of localized air flow patterns on particle concentration distributions as the aerosols are transported through space in the indoor environment.

Important findings about the particulate behavior of aerosol consumer products were that compressed gas propellants appeared to result in a wider distribution of particle sizes than hydrocarbon pro-

pellants, and that the velocity of the aerosol particles decreased with increasing distance from the aerosol spray nozzle. More than 90% of the particles were found to be larger than 25  $\mu\text{m}$ . It was also found that room air ventilation did have an effect on aerosol particle concentration distribution. The particle distribution was stratified so that the particle distribution was densest in the lower portion of the room and more dilute in the upper portions of the room.

A simplified engineering model was developed to predict the mass, momentum, and energy flux over space of aerosol consumer products – critical factors for evaluating aerosol consumer product efficacy. Applying the model, it was found that the spray cone pattern showed a correlation between material properties of the liquids and the spray patterns. The velocity of the aerosol particles in the hydrocarbon propellant driven sprays appeared to be increasing near the spray nozzle. This may have been caused by evaporation of the liquid propellants near the spray nozzle. The velocity peaked at a distance of 20 mm from the nozzle, and then decreased as the distance from the nozzle increased, probably due to air drag. This mechanism appeared to control the atomization process near the spray nozzle.

### Technology Costs

Since the AMSI is not commercially available and must be machined, the costs depend on the individual machine shop. In general, the cost of the AMSI should be below \$1000. The AMSI, in its current form, must be interfaced with a MS with PB or electrospray (or ion spray) capabilities and preferably with MS/MS capabilities. These systems range from \$150,000 to \$500,000, depending on their

sophistication. Once the AMSI/MS is operating, the analytical costs will range from a few tens to a few hundreds of dollars per sample.

The final costs of the PIV system depend on the instrument manufacturer and features of the components. Generally, the cost of a system to measure aerosol dispersion through space is about \$75,000 to \$90,000. The time required to measure aerosol dispersion is considerable since the data interpretation is labor-intensive. Characterization of the aerosol spray pattern requires approximately 1 hour for data collection, approximately 6 hours to calculate concentrations, and approximately 12 hours to calculate velocity distributions.

### Technology Limitations

There are limitations to the tools developed under this project. However, most of these limitations can be overcome with additional research.

The AMSI is applicable only to aerosols that exit the nozzle in a spray form, using either propellant or pump spray systems. Aerosols that are ejected as foams or gels cannot be introduced into the MS by the AMSI. Also, high viscosity aerosols that are released primarily as dry particles, such as spray powders or paints, will quickly contaminate the AMSI and MS during analysis. This limitation will be extremely difficult to overcome, and probably cannot be eliminated with the current AMSI design. These types of products will require a different type of sample introduction method.

Particle size selection with the AMSI is not currently calibrated. Experiments showed that the numbers of smaller particles transferred into the MS from the AMSI are reduced, but it is not possible to

give the range of particles that are being transferred into the MS.

The developed PIV system allows for the determination of two-dimensional structures of full-scale room air flows and particle concentration. Two cameras or holograms are required to measure particle dispersion in three-dimensional space. The current system measures particle velocities within 5% accuracy for particles larger than 100  $\mu\text{m}$ . A newer and faster PIV system would increase speed and simplify fate and transport measurements, allowing smaller particles to be measured with increased accuracy.

### Study Results

The tools and methodologies developed under this research project can be used to better understand aerosol consumer product behavior. Once this understanding is achieved, effective pollution prevention strategies can be designed. Potential pollution prevention strategies include product reformulation, raw materials substitution or more use of pure raw materials, and modification of instructions for users. These data can be obtained by using the tools developed during this research project.

When manufacturers begin using these tools to study their products, they will be able to determine the chemical composition of the products when they reach the use site, and to determine the minimum amount of active ingredients necessary for efficacy. Manufacturers can investigate the effects of product dispersion and the effects of room air movement on dispersion, to better guide consumers on actual use conditions. An understanding of the chemistry of dispersion can lead to reformulations that minimize cross-media transference during use.

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*The complete report, entitled "Application of Pollution Prevention Techniques to Reduce Indoor Air Emissions from Aerosol Consumer Products," (Order No. PB2001-107254; Cost: \$29.50, subject to change) will be available only from*

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