Y/UMTC-0001

Y/UMTC-0001

Y-12

OAK RIDGE
Y-12
PLANT

LOCKHEED MARTIN

CRADA Final Report
for
CRADA Number Y1294-0296

Optical Particulate Emission Monitor

A. C. Miller, Jr., Bruce E. Bernacki
Lockheed Martin Energy Systems, Inc.
Robert J. Nuspliger
Environmental Systems Corporation

October 15, 1995

Approved for Public Release:
distribution is unlimited.

Prepared by the
Oak Ridge Y-12 Plant
managed by
LOCKHEED MARTIN ENERGY SYSTEMS, INC.
for the
U.S. DEPARTMENT OF ENERGY
under contract DE-AC05-84OR21400

MANAGED BY
LOCKHEED MARTIN ENERGY SYSTEMS, INC.
FOR THE UNITED STATES
DEPARTMENT OF ENERGY

DISTRIBUTION OF THIS DOCUMENT IS UNL

Final Report
CRADA No. Y1294-0296
with
Environmental Systems Corporation
for
Optical Particulate Emission Monitor

by

Arthur C. Miller, Jr., Bruce E. Bernacki
Lockheed Martin Energy Systems

and

Robert J. Nuspliger
Environmental Systems Corporation

October 15, 1995

Abstract:

The Oak Ridge Centers for Manufacturing Technology (ORCMT) and Environmental Systems Corporation (ESC) have collaborated on an effort to develop the optical system for an enhanced particulate emission monitor. The purpose of this effort was to assist a small East Tennessee company in perfecting an instrument that would meet or exceed the performance of competing foreign instruments and provide measurement capabilities necessary to assure compliance of Department of Energy facilities and other industrial facilities with expected EPA regulations. The two parties collaborated on design, assembly, and bench testing of the prototype instrument. The prototype system was targeted to have the capability for measuring micron size particles in concentrations as low as 10 micrograms per cubic meter and to have the added benefit of improving sampling statistics (i.e. measurements will be made over larger regions of the stack) over current instruments. Project deliverables were a prototype optical system and characterization data.

Background

Recent studies by the Environmental Protection Agency and the Harvard School of Public Health reported in the Wall Street Journal(1), the New York Times(2) and other publications have estimated that 50,000 to 60,000 deaths per year are caused by particle pollution, which is a far greater number than from any other form of pollution. The New England Journal of Medicine(3) reports that fine particulates less than 2.5 microns in diameter which contain soot, acid condensates and sulfate and nitrate particles are the most damaging contributors to increased lung cancers and cardiopulmonary disease. Present U.S. EPA standards for these emissions assumed much more rapid retirement of older electricity generating plants than actually has occurred, and they are presently monitored by very inaccurate means. As a result this form of pollution is not well controlled, and it is generally expected that the EPA will establish far more rigorous limits in the very near future.

In Europe, Germany has instituted much tighter limits than the U.S. and presently most instruments available for on-line monitoring of such particulates are made there. The purpose of this CRADA was to assist a small East Tennessee business in perfecting an instrument that would meet or exceed the performance of the German instruments and provide measurement capabilities necessary to assure compliance by Department of Energy facilities and industry with expected EPA regulations.

Project Objectives

The prototype system developed was targeted to have the capability for measuring micron size particles in trace concentrations. The desired goal was 0.1 milligrams per cubic meter with a target goal as low as 10 micrograms per cubic meter. The prototype instrument was to achieve this sensitivity through use of higher powered light sources coupled to optimal beam forming and scattered light receiving optics. It was also desired that the instrument have improved sampling statistics (i.e. measurements made over larger regions of the stack) over current instruments. Overall system response time was to be less than two seconds. Finally, the instrument design should allow operation outside the stack, requiring only optical access to the source gas to be measured which greatly lowers maintenance costs, allows the use of high performance light sources, and thus provides an important competitive advantage.

In this project the Ultraprecision Manufacturing Technology Center (UTMC) and ESC were to collaborate on development of the exact optical and electronic system specifications required to meet overall system performance goals. Within ORCMT, the UMTC was to design the custom receiver optics and fabricate the components using single point diamond turning. ESC was to provide the electronic source and receiver signal conditioning equipment and components (laser sources, detectors, power supplies, amplifiers, etc.) and design and fabricate the custom mechanical parts required to assemble the prototype instrument. The two parties then were to collaborate on source selection, component assembly and bench testing of the prototype instrument.

To summarize project objectives:

1. Design prototype source and receiver optical system with 0.1 mg/m^3 sensitivity minimum and target concentrations as low as 10 μg/m^3.
2. Design should allow improved sampling statistics.
3. Design should allow use of high power light sources that can be located outside stack.
4. System response time less than 2 seconds.

Project Results

Initially, two custom designs of the receiver optics were pursued, refractive and reflective. Both involved a folded axicon approach, although the reflective design was ultimately chosen due to the many advantages in materials and auxiliary system integration flexibility. Both designs allowed operation outside the stack, therefore it was possible to use high powered light sources. Laser diodes were chosen and collaboratively evaluated for beam shape and power.

ESC addressed the preamplifier and noise considerations for achieving the desired instrument sensitivity. After design, fabrication, and testing of the prototype optical system, it was then evaluated for performance. Excessive diffractive scatter was found in the diamond machined surfaces which adversely affected the system performance. Various methods of buffing the surfaces were explored, and a redesign involving a single surface was also investigated. These attempts yielded marginal improvements over the original system performance. However, insight gained in testing the system led to a design modification that significantly reduced the effects of stray light.

The modification to the axicon approach involved the use of a reimaging telescope to eliminate stray light and produce the desired sampling volume response. Altering the design to move the peak of the sampling volume to different axial positions proved cumbersome, and measurements did not always meet predictions. As a result, an all spherical design was created with similar selection criterion for stray light rejection. Components for this design were procured, assembled and tested. Except for some artifacts of the rejection criterion, the alternate design produced sampling volume responses equal to the axicon system and proved much easier to modify for different peak locations.

The project design goals and performance results are listed below in the chart titled "Laser-Based Particulate Monitor Design Goals and Prototype Results". The most important parameters were sensitivity, response volume, and low manufacturing cost. As can be seen from the comparison, the most important parameters have been met. Sensitivity of the prototype instrument is more than a factor of two better than the desired goal and can easily be further improved by increasing the optical power to the laser diode. The curves "Axi 2&3 Comp", "Test 1", "Test 2", "Test 3", (Figures 7,9,10,11) in the technical section were plotted from prototype instrument data and show relocatable sampling volume peaks from both axicon and spherical designs. Moving the peak to 2 or 3 M positions was demonstrated, but resulted in low scattering acceptance angles. The spherical design uses moderately priced off-the-shelf components to achieve low manufacturing cost.

Laser-Based Particulate Monitor Design Goals

Parameter	Minimum Goal	Desired Goal	Prototype Results
Sensitivity	0.2 mg/m^3	0.1 mg/m^3	<0.05mg/m^3
Receiver Optics Max Diameter	13.52cm (5.23")	15.24 cm max (6.0") or smaller	15.24 cm
Response Volume	1 cm dia. Over 76.8 cm, peak at 71cm	Total sampling volume within 1 M path length. Peak at 0.5, 1, 2, or 3 M	Sampling volume demonstrated within 1 M path length with peak over 0.5 - 1.2 M range
Response time	2 sec or less	2 sec or less	2 sec
Zero Stability	±1% in 2 hr ±2% in 24 hr	±1% in 2 hr ±2% in 24 hr	Not tested
Span Stability	±2% in 2 hr ±5% in 24 hr	±1% in 2 hr ±5% in 24 hr	Not tested
Operating Temperature Range	-40°C to 60°C	-40°C to 60°C	-40°C to 60°C

Deliverables:

1. 2 Bench-scale prototype optical instruments that were tested and evaluated for detection capabilities

2. Engineering system designs and component specifications for a field instrument

Benefits to DOE

This project has direct benefits to Defense Programs by enabling a commercially produced instrument capable of monitoring particulate emissions from DOE facilities down to trace levels. It also provided benefits in maintaining DOE-DP expertise and capabilities in the demonstration and validation of ultraprecision state-of-the-art equipment. The DOE retains expertise in these critical fields through the fabrication and evaluation of the prototype and can spin-off important optics related patents with possibilities for licensing to ESC. In addition, the project will encourage the development of a commercial infrastructure capable of ultraprecision machining as the production units are ordered and fabrication technology is transferred to private companies.

This project is a continuation of a direct assistance project and DOE User/Deployment Center involvement with ESC at the ORCMT. The direct assistance project was designed to improve the optics of an existing commercial instrument manufactured by ESC. This CRADA extended the technology by incorporating a new laser-based technique with associated novel optical techniques.

Technical Discussion

Introduction

Light collecting systems often require radically different optical surfaces than those commonly found in optical imaging systems. As an example, an optical particulate monitor collecting back-scattered light must probe a representative volume in emission stacks in order to achieve a good statistical distribution of suspended particles. However, ideal imaging systems map object planes into conjugate image planes and can probe only small volumes.

This CRADA involved the design and performance of novel optical collection systems that utilize precision-engineered reflective conical surfaces (axicons) in a telescopic arrangement that map a line in object space onto the detector plane in image space. Such non-spherical surfaces are nearly impossible to fabricate using traditional methods, but can be made easily using the deterministic method of single point diamond turning. In addition to complex optical surfaces, single-point diamond turning also makes possible the precision engineering of reference surfaces useful for pre-alignment of multiple surfaces and rapid assembly of the finished system.

The axicon is a conical refracting or reflecting optical element that can map a line along its generating axis into a point image at finite conjugates. At infinite conjugates, the imaged point is infinitely distant, resulting in collimated light, and all of the conjugate rays make the same angle with respect to the optical axis. This feature can be exploited to collect scattered light with a specific scattering geometry to infer particle density or mass concentration, size, and surface area to name a few characteristics. The design, fabrication and performance of an instrument using reflective axicons is described.

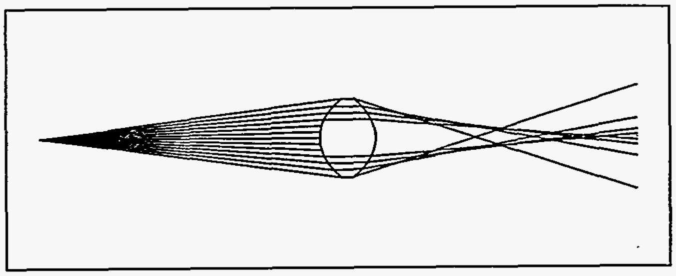


Figure 1. Scattering collector based on an equi-convex lens and central obscuration. Note the caustic (extended focal line) due to the large amount of spherical aberration.

Collecting light scattered at a particular reference angle provides information about the physics of a process. A straightforward method uses a masked lens to admit an annulus of light having the desired scattering geometry, as seen in Figure 1. The collected light can then be focused onto a detector. The drawback to this method is its poor efficiency and the limited scattering volume that can be probed. One exploits a poorly-corrected collection lens to ensure that there is enough spherical aberration to create a large caustic (4) (density of rays from the paraxial focus to the marginal or rim focus) that can probe along the optical axis of the lens. The caustic is sometimes referred to as "the locus of the focus." Two shortcomings are immediately evident with this approach. The first is the reduced throughput of the system due to the masked aperture, and the second shortcoming is the inability to ensure that only those scattered rays having the desired scattering geometry reach the detector.

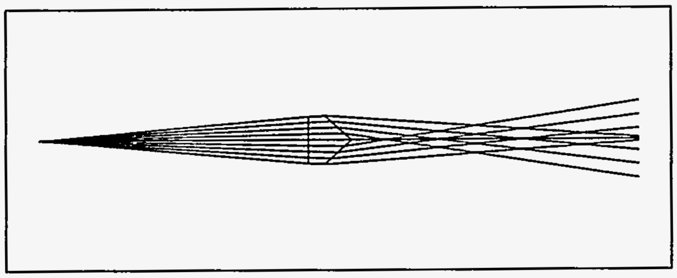


Figure 2. Refracting axicon showing the conjugate relationship between a line along the optical axis and its conjugate object point.

Basic Axicon Theory

The axicon is an alternative and arguably more elegant approach to collecting scattered light. An axicon is a conical refracting or reflecting optical element that can map a line in object space into a point in image space.(5,6) A refracting axicon is shown in Figure 2. Application of Snell's law and some basic trigonometry shows that for small apex angles, the refracted (reflected) ray for infinite conjugates makes the following angle ω' with respect to optical axis:

$$\omega' = (n - 1)\,\alpha. \tag{1}$$

where α is the apex angle measured from the surface of the axicon to the normal of the optical axis. This is a paraxial approximation that is reasonably accurate for apex angles less than 10 degrees. The length of the line focus that begins at the cone of the axicon is found to be:

$$\text{length} = \frac{h}{\omega'} = \frac{h}{(n-1)\,\alpha}\,. \tag{2}$$

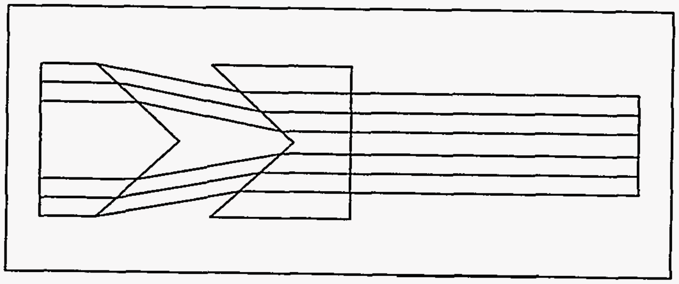


Figure 3. Afocal tele-axicon demonstrating compression of a collimated beam into a smaller diameter annulus.

If two axicons are combined having positive and negative cone angles, the so-called tele-axicon arrangement results. (7) Figure 3 shows an afocal tele-axicon arrangement that finds use in beam expansion or compression in laser machining.(8) The general expression for the refracted (reflected) angle for two axicons in combination is

$$\omega' = (n - 1)\,(\alpha_1 - \alpha_2). \qquad (3)$$

One can see that for the afocal arrangement, the apex angles must be equal and opposite in sign. By choosing the two apex angles appropriately, one can shift the focal line away from the apex of the axicon. Figure 4 shows an example of a shifted line focus.

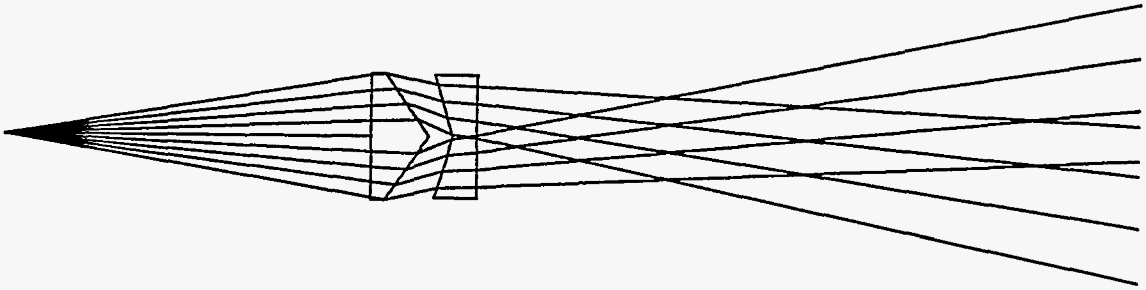


Figure 4. Tele-axicon showing the focal line shifted along the optical axis away from the apex of the second axicon.

Paraxial Ray Tracing For Axicons

First-order system design using paraxial ray tracing is useful for laying out the optical train rapidly. The matrix approach is a methodical implementation of paraxial ray tracing.(9,10) A 2 x 1 column vector is used to specify the height of the input ray with respect to the optical axis, and the optical angle the input ray makes with respect to the optical axis. The optical angle is the product of the geometric angle and the index of refraction in that optical space. Refraction (reflection) and transfer are represented with 4 x 4 matrices. The forms for these matrices are:

$$\mathbf{R} = \begin{pmatrix} 1 & 0 \\ \dfrac{-(n-1)\alpha}{h} & 1 \end{pmatrix}$$

$$\mathbf{T} = \begin{pmatrix} 1 & \tau \\ 0 & 1 \end{pmatrix} \qquad (4)$$

where τ is the reduced distance, t/n, and n is the index of refraction. The refraction and transfer matrices are used for reflective systems by assigning the value of -1 to the index of refraction. The lower-left element of the refraction matrix is analogous to the expression used for optical power in spherical-element refracting (reflecting) optical elements, and its reciprocal, focal length, is equivalent to the expression for the line focus extent shown in Eq. 2. A complication of this analogy requires that one substitute h for whatever number or expression occupies the ray height position in the input ray vector.

Paraxial Design of the All-Reflective Scattering Collector

The approach to designing the collector begins with writing the paraxial expressions for ray height and optical angle after reflection from the first axicon (primary) after collecting light along the optical axis at the design scattering angle, and also the final expression after reflection from the second reflecting axicon (secondary). To ensure only light at the desired scattering angle is collected, infinite conjugates result. A focusing element, in this case, a parabolic reflector, ensures that parallel light is directed onto a detector. In practice it is easier to trace the ray backwards from the secondary, to the primary, and finally, to the optical axis.

After reflection from the secondary for a ray with height h and optical angle 0 (parallel to the optical axis), the ray vector can be found to be:

$$\mathbf{r}_s = \begin{pmatrix} h - 2\alpha_s t_1 \\ 2\alpha_s \end{pmatrix} \qquad (5)$$

where t_1 is the separation between the primary and secondary axicons. After reflection from the primary, the ray vector is:

$$\mathbf{r}_p = \begin{pmatrix} h - 2\alpha_s t_1 + 2(\alpha_s + \alpha_p) t_2 \\ 2(\alpha_s + \alpha_p) \end{pmatrix} \qquad (6)$$

where t_2 is the distance from the primary to the scattering plane. One can now form several equations with design values substituted to determine the instrument unknowns. For example, the diameter of the instrument, which may be constrained by size limitations, along with the desired scattering angle, sets the extent of the line focus along the optical axis. In this case, the diameter was limited to 150 mm. Also, to maximize scattering volume, one must choose the desired working distance or stand-off that is determined by the sum of the apex angles of the tele-axicon. The desired working distance in this case was 500 mm. Finally, one can choose a separation distance between the primary and secondary axicons to limit the overall length of the instrument. In the case of the all-reflective collector, a very compact design is possible. Here, 50 mm was chosen as the design goal.

Computer Design of Axicon Instrument

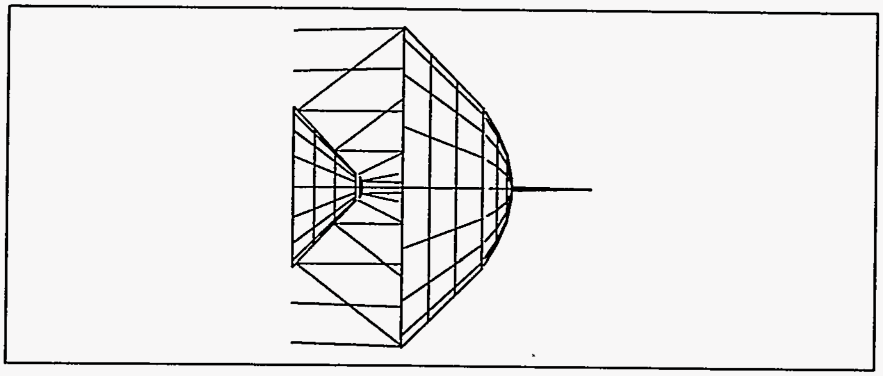


Figure 5. Layout drawing of the finished axicon collector showing parallel rays at the desired scattering angle imaged at infinity, then refocused onto the detector surface using the telescope.

ZEMAX-EE, a commercially-available lens design program was used to produce an optimized design of the scattering instrument. The axicon was modeled as a conic section having a very small radius of curvature, and conic constant related to the apex angle of the axicon. Recall that the sag equation of a general conic section is:

$$z(r) = \frac{C r^2}{1 + \sqrt{1 - (1 - \kappa) C^2 r^2}} \qquad (7)$$

where κ is the conic constant, and C is the curvature of the element. To model an axicon using the above sag equation, the following equality is employed:

$$\kappa := -\left(\frac{1}{\tan^2\theta} + 1\right) \qquad (8)$$

where θ is the axicon cone angle. The curvature is set to something smaller than $0.1\ \mathrm{mm}^{-1}$ with the sign of the curvature denoting whether the axicon is positive or negative. The correct angles are found by setting up input rays at the desired scattering angle, and using real angle solves to ensure that the rays exiting from the secondary axicon are parallel. A telescope is then used to bring the parallel rays to a focus on the detector surface. The finished axicon scattering instrument is shown in Figure 5. By using a two element telescope to focus the rays, only shallow rays reach the detector, reducing Fresnel losses at the detector window and active surface of the detector. Additionally, stray light rejection is enhanced because the detector doesn't "see" the scattering volume.

The performance of the finished collector can be modeled by placing a point source along the optical axis and using the encircled energy function to quantity the amount of light within a circle having the same diameter as the detector. The encircled energy is then integrated and plotted as a function of source distance. The complete predicted response curve is shown in Figure 6. The source is measured from the base of the secondary axicon in units of millimeters. The response is normalized with respect to the maximum value. Note that the 10% points are approximately 450 mm wide.

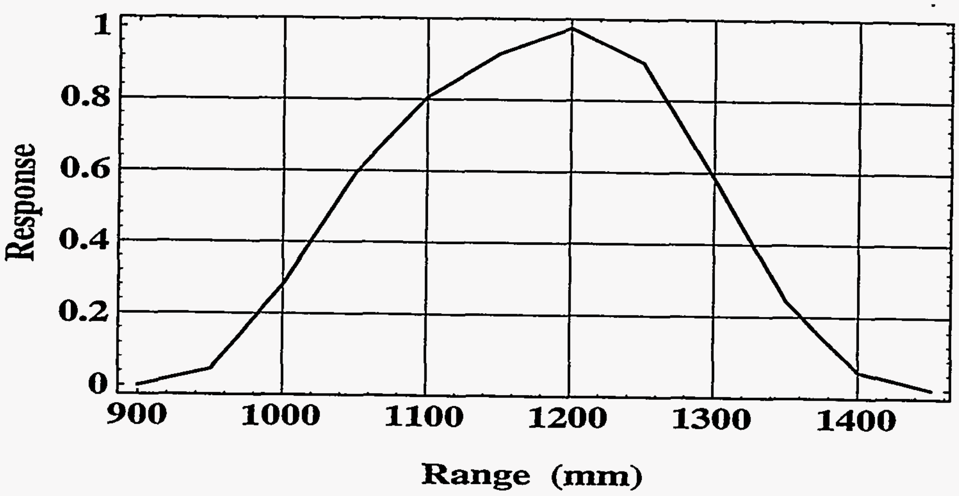


Figure 6. Normalized response of the axicon scattering collector versus distance measured from the base of the secondary axicon.

The axicon can be used to map a line in object space into a point in image space. This is exactly the behavior sought when constructing a scattering collector, since a volume in scattering space must be probed to obtain adequate statistics. In this approach, a telescope-like arrangement of two axicons is employed so that the focal line can be shifted away from the instrument to facilitate scattering collection in effluent stacks. The finished design images scattered rays at the desired scattering angle at infinity. To develop a signal, a reflective telescope re-images the parallel rays onto a finite-sized detector using a two-bounce configuration. The focusing telescope enables the detector to face away from the scattering angle to eliminate stray light effects, and also lessens the incident angles at the detector window and active surface of the detector, which reduces Fresnel losses. Figure 7 shows the measured response to the axicon design reconfigured to move the peak sampling volume to two different axial positions.

An alternative, all spherical design was also investigated for comparison to the axicon approach. Similar design constraints were placed on the imaging properties of the system. The predicted response is shown in Figure 8. Several artifact peaks are noted and result from stray light rejection features of the design. Figures 9, 10, and 11 show the bench prototype measured response at various peak locations for the alternate spherical design.

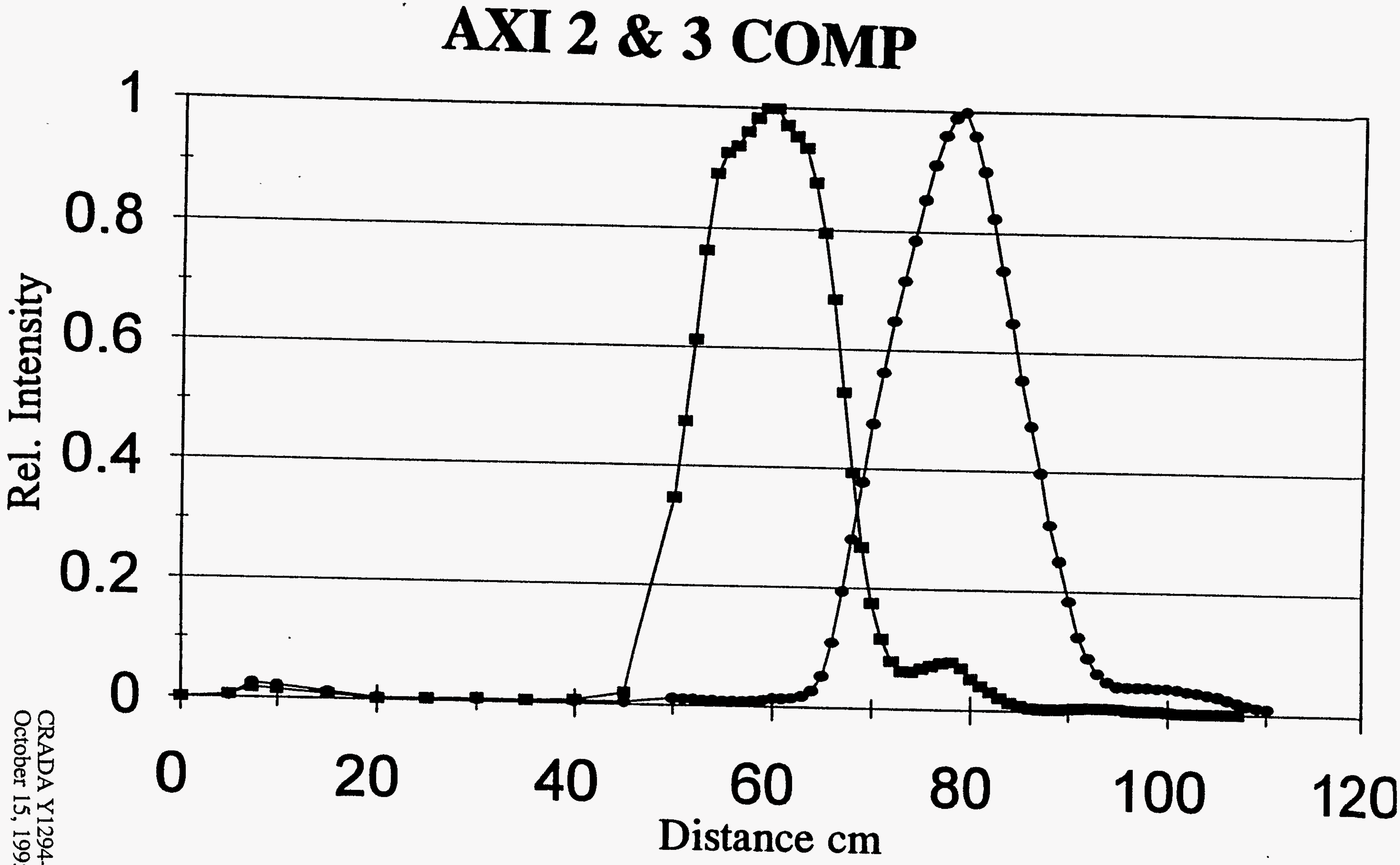
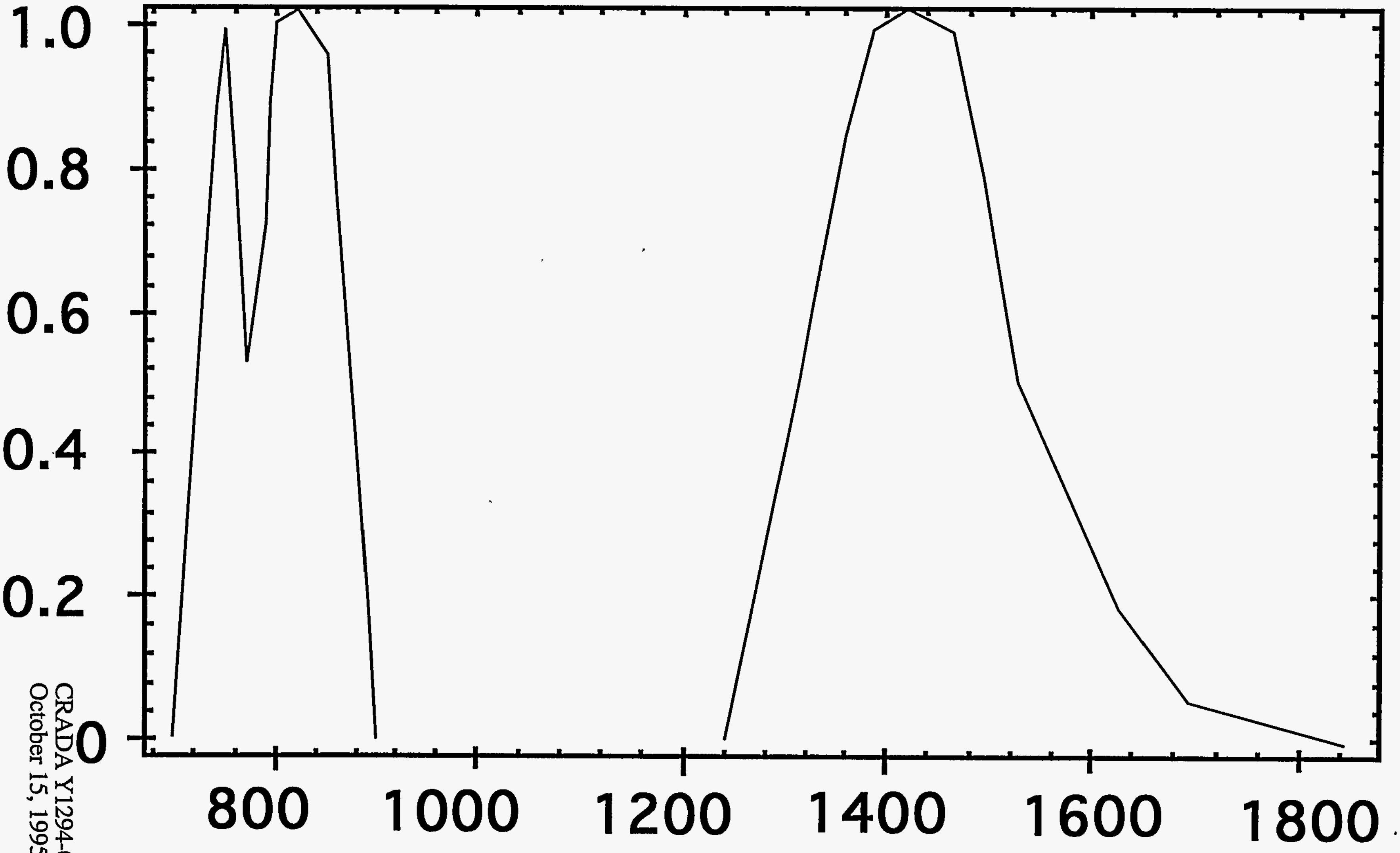


Figure 7. Axicon bench prototype response at different axial positions



Note: All Peaks normalized, and
0 = flat surface of secondary

Figure 8. Spherical Design Predicted Response

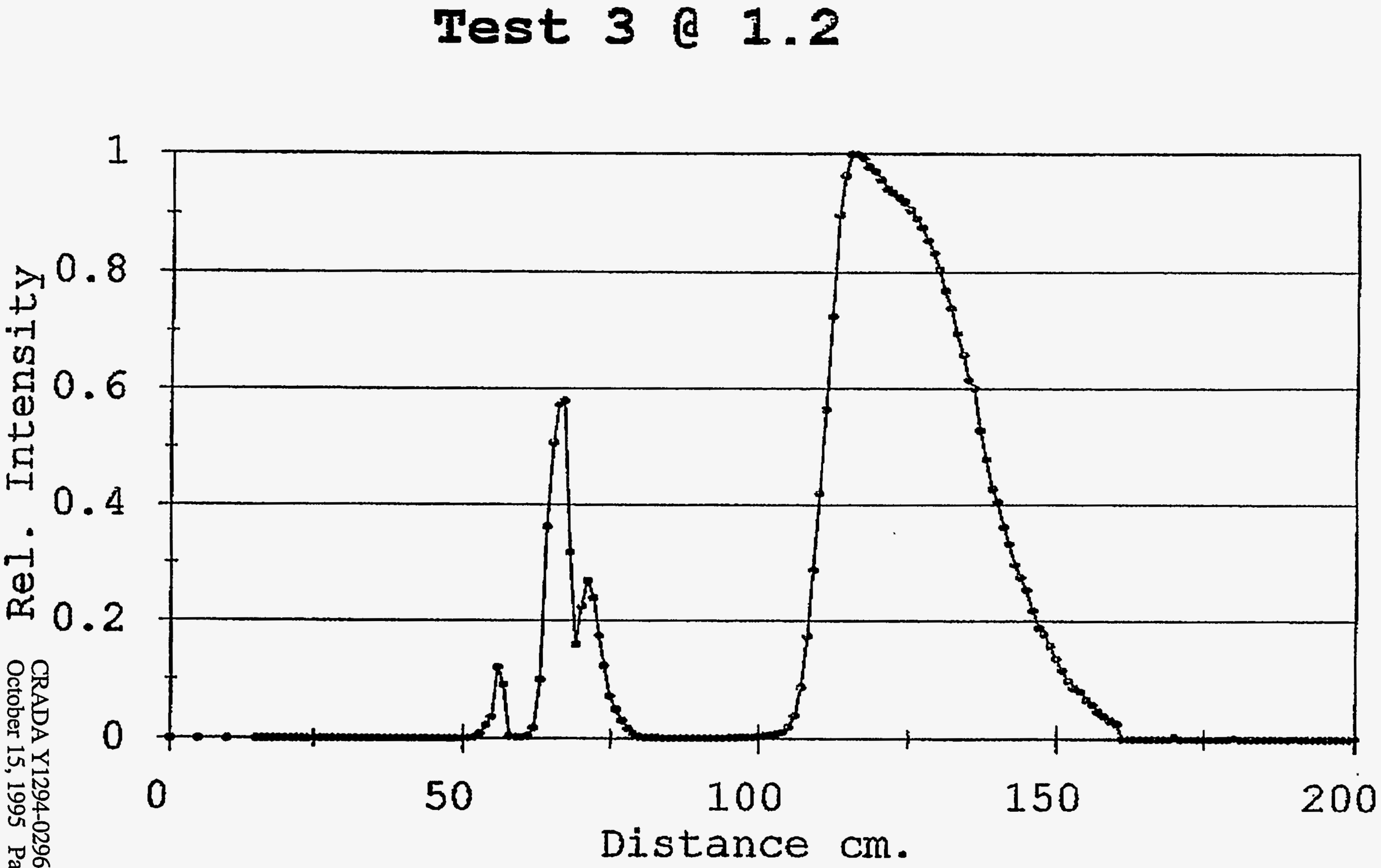


Figure 9. Spherical bench prototype response at 1.2 M

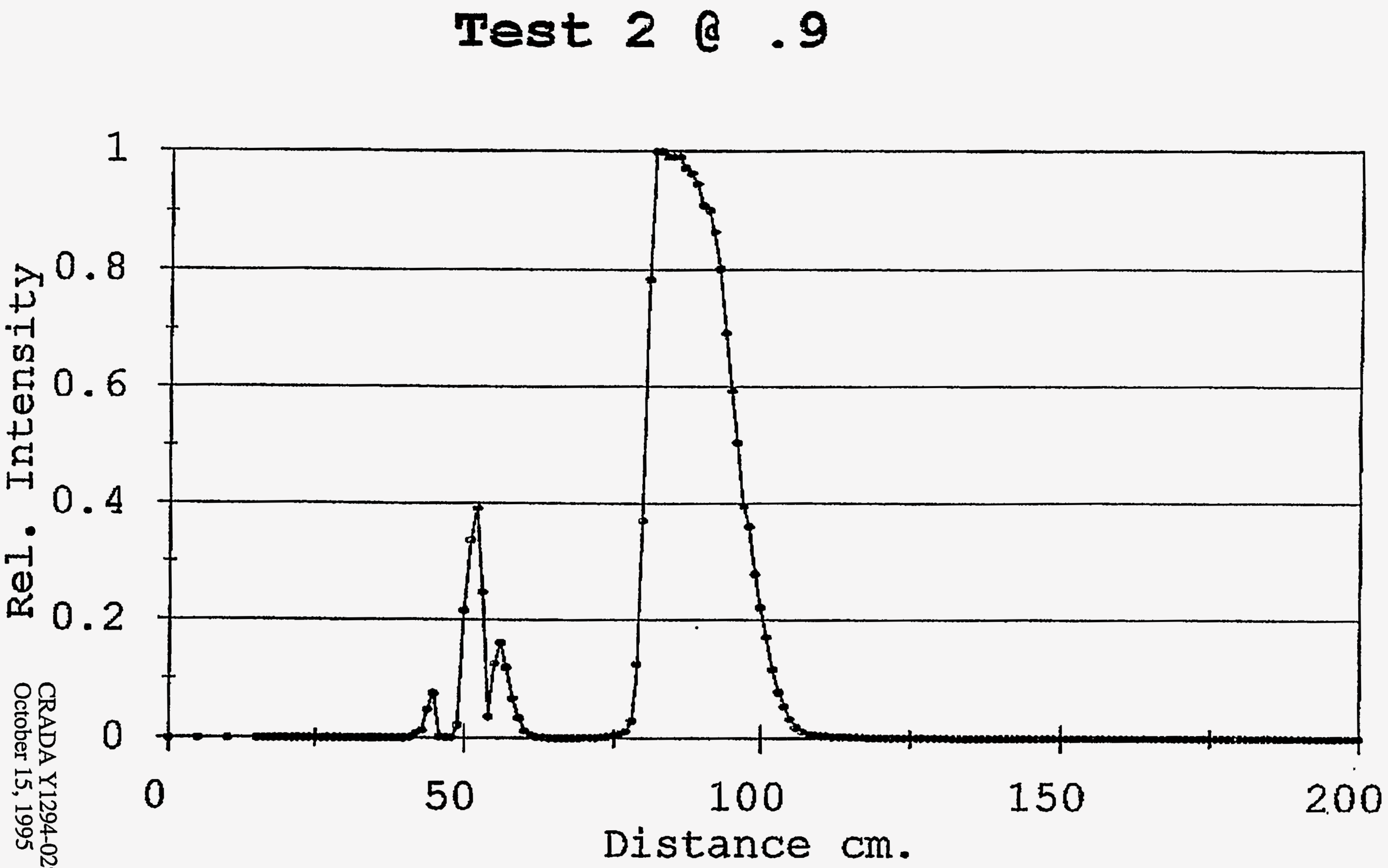


Figure 10. Spherical bench prototype response at 0.9 M

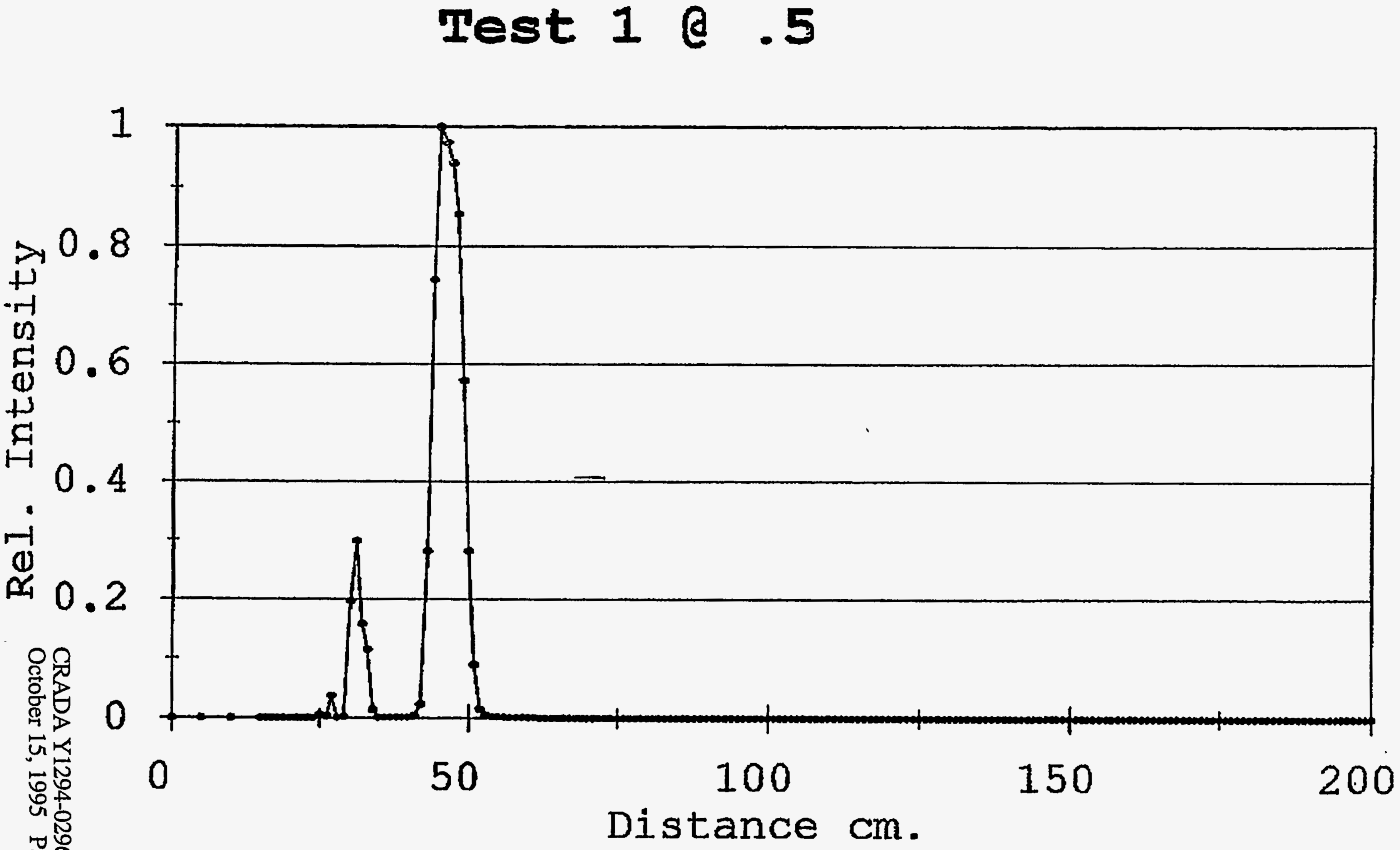


Figure 11. Spherical bench prototype response at 0.5 M

Inventions

An invention disclosure was filed with LMES concerning the receiver optical design prior to signing the CRADA agreement. This device has licensing possibilities with ESC for future instrument designs. Also, an invention disclosure is being filed describing an alternate design that was developed jointly during the CRADA.

Commercialization

The CRADA project will result in direct commercialization of the prototype instrument by ESC to meet foreign competition. Further collaboration is on-going with ESC via the DOE User/Deployment Center association.

Field testing of the instrument is expected to begin in the first quarter of 1996, with release to production occurring in the third quarter of the year. The projected increase in sales for the next 5 years, as a result of this development is expected to exceed $4.6M.

It is further believed that this sales increase will result in the additional full-time employment of 5-6 people within ESC as well as another 7-9 local area job increases in subcontract work for machine parts, printed circuit boards, etc.

Conclusions

The prototype optical instrument developed under this CRADA meets or exceeds the target specifications for the detection of particles in low concentrations, as well as for measurements at various (adjustable) sampling regions external to the system itself. Work is presently continuing via DOE User/Deployment Center activity to determine optimum methods for instrument calibrations and to define more completely technical specifications such as zero, span stability, and limit of detection.

Principal investigators:

Contractor

Arthur C. Miller, Jr. , Manager
Ultraprecision Manufacturing Technology Center
P.O. Box 2009
Oak Ridge, Tennessee 37831-8039
(615) 574-9411 FAX (615) 574-9407

Participant

Robert Nuspliger
Environmental Systems Corporation
200 Tech Center Drive
Knoxville, Tennessee 37912
(615) 688-7900 FAX (615) 687-8977

---

(1) "Studies Say Soot Kills up to 60,000 in U.S. Each Year," Wall Street Journal, July 18, 1993.
(2) "Studies Say Soot Kills Thousands a Year," New York Times,July 19, 1993
(3) "National Air Pollutant Emission Trends, 1900-1992", EPA-454/R-93-032, October 1993
(4) Welford, W. T., Aberrations of optical systems, (Adam Hilger, Boston, 1986), p. 111.
(5) McLeod, J. H., "The Axicon: A New Type of Optical Element," JOSA, 44 (8), 592-597 (1954).
(6) McLeod, J. H., "Axicons and Their Uses," JOSA, 50 (2), 166-169 (1960).

(7) Bickel, G., G. Häusler, and M. Maul, "Triangulation with expanded depth of range," Opt. Eng., 24 (6), 975-977 (1985).
(8) Rioux, M., R. Tremblay, and P. A. Bélanger, "Linear, annular, and radial focusing with axicons and applications to laser machining," Appl. Opt., 17 (19), 1532-1536 (1978).
(9) Gerrard, A. and J. M. Burch, Introduction to Matrix Methods In Optics, (Dover Publications, New York, 1994).
(10) Brouwer, W., Matrix Methods In Optical Instrument Design, (W. A. Benjamin, New York, 1964).

Distribution:

D.	E.	Beck
B.	E.	Bernacki
J.	L.	Cook
E.	L.	Epple
C.	F.	Leitten
A.	C.	Miller
R.	C.	Riepe
S.	G.	Snow
R.	S.	Steele

R. J. Nuspliger
Environmental Systems Corporation