
**Innovations Deserving
Exploratory Analysis Programs**

I **DEA**

NCHRP IDEA Program

Prototype Development: Automated and Continuous Aggregate Sampling and Laser Targeting System

Final Report for
NCHRP IDEA Project 168

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NCHRP IDEA Program

Final Report

Project NCHRP 168

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Aggregate Sampling and Laser Targeting System**

Prepared for the NCHRP IDEA Program

Transportation Research Board

The National Academies

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LIST OF ACRONYMS AND ABBREVIATIONS

AASHTO	American Association of State and Highway Transportation Officials
AIR	acid insoluble residue
ASG	apparent (true) specific gravity
BSG	bulk specific gravity
CCD	charged coupled detector
EMR	electromagnetic radiation
HMI	Human Machine Interface
IDEA	TRB Innovations Deserving Exploratory Analysis Program
KSDOT	Kansas Department of Transportation
LIBS	Laser-Induced Breakdown Spectroscopy
MLR	multiple linear regression analysis
NCHRP	National Cooperative Highway Research Program
Nd:YAG	neodymium-doped yttrium aluminum garnet crystal
NYSDOT	New York State Department of Transportation
ODOT	Ohio Department of Transportation
OKDOT	Oklahoma Department of Transportation
PADOT	Pennsylvania Department of Transportation
PC	Principal Component
PCA	Principal Component Analysis
PLS	Partial Least Squares Regression
QC	quality control
SLT	Sampling and Laser Targeting System
SLTDAM	SLT Data Analysis and Modeling System
SLTOPS	SLT Operator System
SSD	saturated surface dried specific gravity
TPF	Transportation Pooled Fund
VAD	Value of Apparent Distinction

EXECUTIVE SUMMARY

Current processes for quality control (QC) in the highway construction industry are time-consuming, highly inefficient and provide considerable risk to the hot mix asphalt and portland cement concrete production industry. Hot mix asphalt and portland cement concrete generally produce and lay down final pavement products prior to receiving quality control testing results. The ramifications of test failures after the pavement is in place are financially and administratively burdensome to the producers, the contractors, and the transportation agencies charged with ensuring that funds to construct and maintain the highway infrastructure are used efficiently. QC issues in the industry are further aggravated by the poor precision associated with many of the sampling and acceptance tests employed by the industry and the skill of technicians conducting such tests.

The research described in this report presents the activities and results associated with the development of a laser scanning prototype device, referred to as the Sampling and Laser Targeting System (SLT). The SLT provides the potential means to rapidly classify aggregates used in highway construction. This classification process can be employed to:

- Quantify specific engineering properties (e.g., specific gravity, acid insoluble residue, and Micro-Deval loss),
- Identify and/or quantify the presence and amounts of deleterious materials present (e.g., reactive aggregates and cherts),
- Determine whether aggregate types or quality are changing during production, and
- Determine the source material or sources of blended production materials.

The process makes use of the high-powered laser that couples with and excites atoms present in the microstructure of target aggregate materials. This atomic excitation process induces the release of electromagnetic radiation that is unique to the aggregate material targeted. As a result, it is possible to “fingerprint” aggregates based on the specific wavelength pattern emitted by the laser-induced emission. The whole process is referred to in the scientific literature as Laser-Induced Breakdown Spectroscopy (LIBS). Once a “fingerprint” is made of an aggregate of known quality or type, it is possible to document that fingerprint and use it as the basis for determining whether an unknown aggregate is the same as the known aggregate or not. By developing a database of aggregate “fingerprints” with varied properties, it is possible to classify an unknown aggregate by comparing it to the known database to determine which aggregate material (fingerprint) it most closely resembles. It is also possible to calibrate aggregate “fingerprints” to enable the measurement of engineering properties such as specific gravity, acid insoluble residue, Micro-Deval loss, etc.



FIGURE 1 Operator pouring aggregate sample into SLT Laser Scanning System.

The “fingerprint” described above is a spectral chemical fingerprint. It is a composite analysis of approximately 14,000 individual light-intensity measurements (visible and nonvisible light) emitted during the laser-aggregate coupling process. To make effective use of these measurements, mathematical categorization of the data is undertaken with the use of chemometric modeling. Chemometric modeling is a multivariate modeling process, unfamiliar to most highway engineers or material analysts. Nonetheless it is a powerful tool that can be employed with the assistance of the proper software to analyze and categorize spectral fingerprints.

The research conducted under this NCHRP 168 effort is a Type 2 IDEA Program. A Type 2 IDEA effort is designed to support the development of prototype systems for the implementation of technologies with proven technical concepts. The concept for this Type 2 effort was validated under NCHRP IDEA Project 150 (*1*).

The NCHRP IDEA Project 168 effort involved the design and fabrication of a prototype SLT, the development of software capable of operating the system and processing, through chemometric modeling, the large quantity of data generated during the scanning process to provide near real-time data turnaround. A photograph of an operator pouring aggregate into the SLT prototype is shown in Figure 1. The aggregate in the bucket flows down through a materials flow chute while a laser fires semi-continuously at the flowing material. The visible and nonvisible light released in the process is resolved into spectra and electronically transmitted to a computer, where the software captures the data and generates models used to classify and identify the material and its properties.

During the course of the study aggregate samples were collected from a number of state agencies, including Kansas, Oklahoma, New York, Pennsylvania, and Ohio for testing and evaluation. [These agencies are also currently participating in a more extensive three-year Transportation Pooled Fund Study to evaluate the technology: Transportation Pooled Fund Study TPF 5(278): “Real-Time Laser Scanning of Aggregate Materials in Highway Construction for Quality Control Monitoring.”] While the bulk of the NCHRP IDEA 168 effort focused on the physical fabrication and integration of the SLT system, the scanned aggregates and the feedback provided by the results of the chemometric modeling procedures employed were used during the course of the research to modify the hardware and software associated with the system and to provide an initial examination of the effectiveness of the process.

Technical research findings were as follows:

- The SLT prototype system developed during the course of this study was capable of routine analysis of approximately 8 to 12 aggregate samples on a daily basis, and capable of scanning bulk aggregate samples in near real time.
- Emission spectra recorded [at wavelengths ranging from 200 nanometers (nm) to approximately 980 nm, derived from averaging spectra generated by firing 1,500 individual laser shots from a high-powered, pulsed neodymium-doped yttrium aluminum garnet crystal (Nd:YAG) laser at aggregate samples] provided the means to generate data that could discriminate among aggregate samples tested in this research effort.
- Multivariate (chemometric) calibration models and validation tests on these models, developed to predict values for acid insoluble residue (AIR), bulk specific gravity, saturated surface dried specific gravity (SSD), apparent specific gravity, absorption, Micro-Deval, approved materials, D-cracking, and percent chert, yielded very promising results.
- The efficacy of such models is dependent on the calibration procedures employed in the process and in particular the heterogeneity of the aggregate test sample set.
- This heterogeneity of aggregate samples provides a great deal of information that must be incorporated into chemometric models to provide the information necessary to develop accurate predictive models.
- The relatively small number of samples tested to date and the large variability in the types of samples tested limited the accuracy of the validation test predictions during this investigation.
- Additional software improvements that provide intensity normalization and drift corrections procedures as well as spectral outlier detection will improve modeling resolution.

It was concluded from these findings that

- Laser scanning in near real-time of aggregate materials is a technology capable of significantly improving the manner in which aggregate quality control procedures are employed by the industry, altering the paradigm of aggregate monitoring established in the early 20th century.

- The SLT prototype developed during the course of this investigation provides a system capable of processing aggregate samples and can be operated by material technicians with no special training.
- The development of the technology will require establishing suitable and expanded laser-induced spectral information databases for target aggregates of interest, with sufficient numbers and types of sample to properly characterize the target property.
- Improvements in data analytical techniques still being evaluated will further assist in resolving the spectral information generated during the laser scanning process and improving model predictions of aggregate properties.

INTRODUCTION

IDEA Product

The product described in this report is a laser scanning system that provides rapid classification of aggregates used in highway construction. The system, referred to as the SLT, functions as an automated real-time aggregate quality control inspection tool. The SLT can be used by a materials analyst to sample and scan-screen bulk aggregate materials to determine whether the targeted material complies with existing specifications. (Based on these scanning results, the analyst can then assess whether or not additional, specification-linked laboratory testing of the aggregate material may be required. To this end, the SLT system has been referred to by some as a "Smart Tester." Such a tool can assist in prioritizing laboratory QC resources to focus on aggregates of questionable quality.)

The SLT system components are contained in a 50 by 75 by 100 cm (2 by 3 by 4 ft) high cabinet, shown in Figure 1. The cabinet houses a laser, supporting power supply, optical components, material flow equipment, and specialized software to scan and characterize the aggregates introduced into the system. This process is accomplished by introducing a bulk aggregate sample between approximately 10 to 15 liters (2.6 to 4 gallons) into the SLT, where a pulsed laser beam is focused on the aggregate particles. This beam induces a high-temperature plasma that excites electrons in the atoms and molecules comprising the aggregate transitioning the excited electrons to higher energy level. This transition is short-lived (microseconds) and when the electrons return to their ground state, electromagnetic radiation is released with distinct wavelength patterns. These wavelength patterns can be detected and provide information on the subatomic, atomic, microscopic, and macroscopic structure of the aggregate. The wavelength patterns can be categorized, through the process of chemometric modeling, to identify the type, source and engineering material properties of the targeted aggregate. (It is convenient to think of chemometric modeling as a form of pattern matching, where patterns of aggregate with specific properties are compared to unknown aggregates to categorize the unknown sample.)

Report Content

The remainder of this report is divided into the following sections. The first section, Concept and Innovation, describes the principles and features of the laser scanning system. The second section, SLT Prototype, outlines the SLT equipment and its operating procedures. The third section, Scanning Results and Analysis, describes scanning results obtained with aggregate samples received from the New York State Department of Transportation (NYSDOT), Kansas DOT (KSDOT), Oklahoma DOT (OKDOT), Ohio DOT (ODOT), and Pennsylvania DOT (PADOT). This section is followed by the Findings and Conclusions section, which provides a concise listing of the major findings and conclusions of the research effort. The last section, Plans for Implementation, provides a description of the continuing efforts being undertaken to develop the technology. The main body of the report is followed by an Appendix that contains an AASHTO Draft Standard Recommended Practice that provides guidance on the purpose and operation of the SLT laser scanning system. The practice is entitled "Rapid Classification of the Type and Engineering Material Properties of Highway Aggregates Using Laser Scanning and Multivariate Modeling." This draft will be submitted to the AASHTO Subcommittee on Materials Testing for review at a future date.

CONCEPT AND INNOVATION

The rapid laser scanning process and the equipment developed and described in this report introduce a means to provide quality control screening in near-real time during aggregate processing or pavement production. The process described requires no special sample preparation and provides the means to characterize aggregate type, quality, source information, and engineering material property data. Materials testing personnel with nominal training will

be capable of maintaining and operating the equipment. Classification and characterization is achievable with the use of bulk aggregate laser scanning equipment described herein that can be deployed in the laboratory or in the field and specially developed software capable of processing large quantities of spectral data, which can be continuously analyzed. The system is designed so that unknown aggregates introduced into the system can be scanned within minutes and engineering property results or aggregate classifications generated shortly thereafter.

The scanning system employs a high-powered pulsed laser that excites the atoms in the aggregate material, resulting in the release of electromagnetic radiation with unique spectral lines and patterns. The laser scanning process is referred to as laser-induced breakdown spectroscopy (LIBS). The unique spectral patterns generated in this process can be equated to fingerprints that reveal information about the underlying microstructure of the target aggregate material, and can be used to assess similarities and differences between aggregates. A spectral pattern generated during scanning from an Oklahoma limestone sample is shown in Figure 2. The abscissa axis contains the emission wavelengths and the ordinate axis the intensity of light at each corresponding wavelength recorded by the spectrometer.

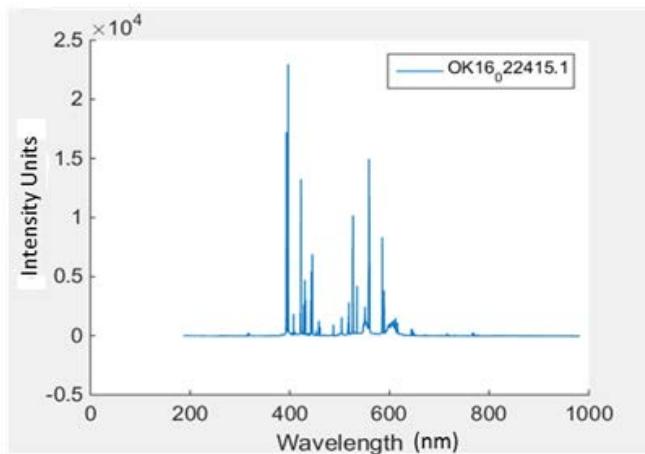


FIGURE 2 Oklahoma limestone spectral pattern.

The spectral patterns of aggregate materials are highly complex and typically contain approximately 14,000 different wavelengths and intensities. To discriminate between and among the spectra patterns generated by the variety of aggregates tested, special mathematical multivariate modeling techniques (chemometric modeling) are employed. These techniques provide the means to discriminate between observed spectra and to regress the spectra against engineering property data. This procedure is accomplished by establishing a database of spectra of known aggregates with known engineering properties. This database can then be used to compare the spectra of unknown aggregate materials with the known materials (in the database). This comparison process provides the means to classify the unknown aggregate or predict the engineering properties of the unknown aggregate materials. Due to the heterogeneity inherent in aggregate particles, suitable characterization requires a sufficient number of laser shots to provide an accurate representation of the spectral pattern associated with the target aggregate. The spectral emission pattern shown in Figure 2 is an average of 1,500 laser shots.

The development of a rapid aggregate laser scanner required the design and fabrication of a new system that could within minutes target representative size aggregate samples with a high-powered laser capable of firing many laser shots in a short time interval and collect and process the spectral emission patterns generated using multivariate chemometric models. A conceptual representation of the SLT process concept is shown in Figure 3. This schematic shows an Nd:YAG laser [The type of laser used in the SLT is an Nd:YAG (neodymium-doped yttrium aluminum garnet) laser; Nd:Y₃Al₅O₁₂ is a crystal that is used as a lasing medium for select solid-state lasers] emitting a high-powered laser beam at a wavelength of 1064 nm directed through a focusing lens and a target orifice. The target orifice opens into a

material flow chute, through which the aggregate sample migrates. The high power associated with the laser generates a plasma that emits light back out of the target orifice. This light (visible and nonvisible) is collected and transported in an optical fiber to a spectrometer and charged coupled detector (CCD). The spectrometer resolves the light into its component wavelengths and the CCD transfers the information electronically to a computer for storage and analysis.

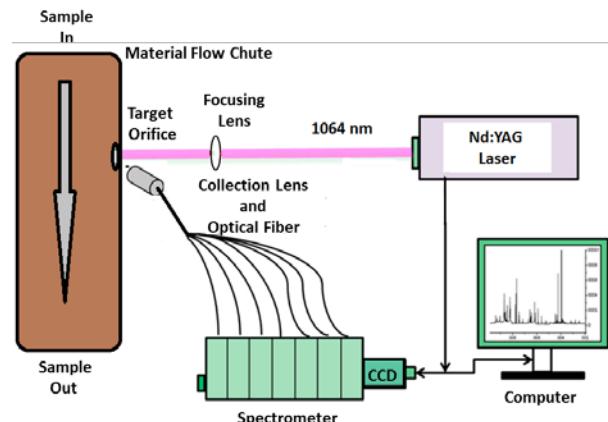


FIGURE 3 SLT LIBS process equipment concept.

SLT PROTOTYPE

Equipment Arrangement

The new system requirements outlined above culminated in the design, fabrication and patenting of the Sampling Laser and Targeting System (SLT), shown in Figure 1. This figure provides a view of the SLT housing. A more detailed representation of the SLT internal equipment configuration is shown in Figure 4.

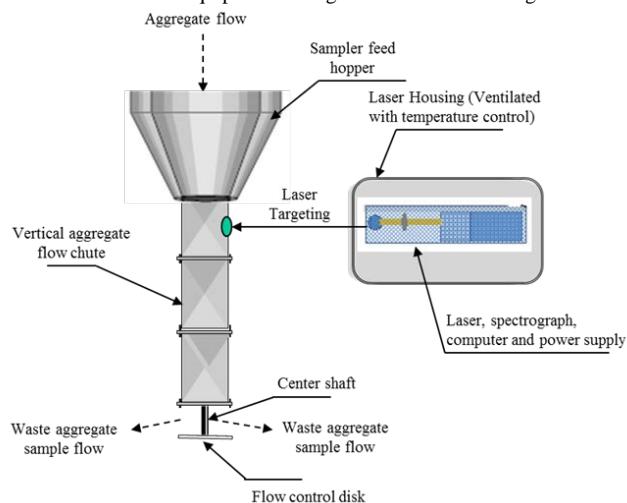


FIGURE 4 SLT equipment configuration: US Pat. 8,902,422 B2 Bulk Sampling and Laser Targeting System.

The SLT is divided into two major compartments: (1) material flow and (2) laser optics. The material flow compartment (located in the left side of the machine housing) consists of a material flow chute (or vertical aggregate flow chute) and the flow control disk, shown in Figure 4. The flow chute and flow control disk provide the means to control bulk material flow in a manner that provides for a uniform flow passed the target orifice. The target orifice is a small hole, located in the side of the flow chute, strategically located to permit the laser beam to pass through the flow chute wall. Aggregate flow control is provided by the flow control disk, located at the bottom of the flow chute. The flow control disk can be lowered (to open the chute to flow) or raised (to close off flow). It is connected to a central vertical shift with tines (narrow and short metal rods), extended horizontally out from the center vertical shaft and spaced at short intervals throughout the vertical shaft length. The central shaft and the flow control disk rotate and the rotating tines and disk assist in imparting a circular motion to the aggregate material in the chute. Aggregate free fall is prevented by the resistance provided by the flow control disk, which prevents material from moving too quickly through the chute. As a result, the aggregate particles are pressed tightly against the wall of the flow chute providing a nearly uniform focal distance from the laser outlet to the migrating aggregate particles, minimizing focal length variability during SLT system operations. There will be some inevitable variability due to the heterogeneity in particle shapes and sizes; however, such variability is mitigated by the large number of laser shots (n) and the averaging of spectra, which takes account the inherent randomness of the system.

The laser beam in the laser-optics compartment, located on the right side of Figure 4, is where the laser and optical equipment, described in detail below, is contained in a separate housing. To exit the optical equipment side of the housing, the laser beam passes through a quartz window and subsequently passes through a pressurized dust suppression system, prior to reaching the targeting orifice and aggregate material. The emission spectra generated by the laser energy travels back through the orifice and quartz window, along the same line as the laser beam, and is captured by an optical fiber that transmits the light to a spectrometer.

Additionally, a dryer is deployed in such a manner as to blow very hot air (in excess of 150°F) directly at the target orifice if necessary. The dryer is activated if wet aggregate is introduced into the flow chute. When such is the case, aggregate flow may be temporarily halted between laser shots (for 1 to 3 seconds) to permit drying of aggregate particles situated behind the target orifice prior to impact by the laser beam.

Data Communications

Repeated laser shots at moving aggregate generate a large quantity of data. Each shot represents a spectral image containing approximately 14,000 wavelengths and corresponding intensities. The data generated have two primary purposes: (1) immediate feedback to the operator regarding the stability of machine operation and (2) input to multivariate chemometric models that provide the means to determine the aggregate variable of interest (e.g., type of aggregate or engineering property).

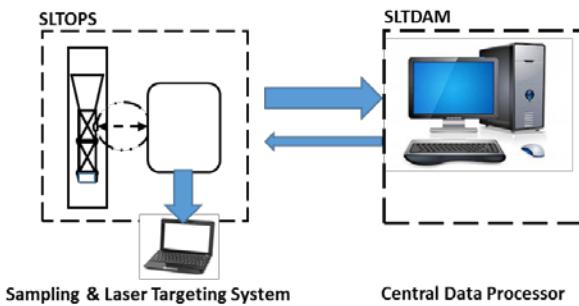


FIGURE 5 SLT data communication system.

The SLT prototype design manages the data in two integrated data management systems. The first is physically located at the SLT and is referred to as the SLT Operator System (SLTOPS). This system provides direct information to the operator concerning the operating conditions of the system and the results of the laser scans. The

second system is referred to as the SLT Data Analysis and Modeling System (SLTDAM). This system is located at a remote data processor, which has the means to import spectral data, collected and stored in the SLTOPS, and transmit these data to chemometric models located at the central data processor. The chemometric models analyze the data and return the relevant engineering information to the operator's SLTOPS system, to define the nature of the targeted material. A summarized schematic of this data communications system is provided in Figure 5.

Multivariate Chemometric Models

Most mathematically derived models used by highway or materials engineers focus on univariate analysis. In univariate analysis, one independent variable is used (at one time) to predict the output (value) of one dependent variable. For example, traffic count or truck traffic, one independent variable, is typically used to predict the service life of a pavement, one dependent variable. Similarly, water-cement ratio is used as a uni-independent variable to predict the value of one uni-dependent variable, Portland cement concrete strength.

In multivariate analysis more than one independent variable is used to describe a dependent variable. For example, one might surmise that other variables besides traffic count might influence the service life of a pavement. These other variables could include average annual temperature, annual precipitation, number of freeze-thaw cycles per year, type of pavement (asphalt or concrete), thickness of pavement, the thickness of the subbase, type of aggregate in the subbase, etc. While there are various quantitative techniques that mathematicians, scientists, and engineers have employed in the past, most notably multiple linear regression analysis (MLR), most of the applied techniques suffer from the problem of collinearity (i.e., the variables are intercorrelated) (mathematically, this implies that the variables are linearly dependent). Practically this means that variables such as annual temperature, freeze-thaw cycles, and annual precipitation are not independent of one another and provide analogous information. Multivariate analytical techniques such as MLR, however, have no way of adequately compensating for this problem and treat each of the variables as if they were independent. In complex multivariate systems (e.g., predicting the service life of pavements), MLR modeling comes up short. As a result, historical attempts at multivariate analysis in complex systems using MLR have met with little success. (The authors surmise that this is a primary reason why multivariate modeling has not been successfully applied in prior pavement design or performance projections.)

To analyze spectral data generated by the LIBS process, with each laser shot containing approximately 14,000 different wavelengths and intensities, it is impractical to employ anything but multivariate analysis. In these spectra there are a total of 14,000 variables with (no doubt) many intercorrelated. This is hardly a task for univariate or multiple linear regression analysis. The preferred methods employed in the analysis of complex system such as this are unfamiliar to most highway or materials engineers. These methods are referred to as "projection methods" or "bilinear projection methods". The strength of these methods rests on their capability of overcoming the problem of collinearity. [This is accomplished by generating orthogonal eigenvectors through the multidimensional data that highlight the factors (latent variables) that are linearly independent, minimizing the influence of variables that exhibit collinearity.]

One of the areas of rapid growth in recent years has been the use of these projection methods in the field of chemical computation or chemometrics. Almost all chemical systems are multivariate in nature and as a result chemometrics, in almost all cases, requires multivariate analysis, and projection methods are the preferred approach. (Since these projection methods require extensive computation, their growth in application has paralleled the growth of desktop and laptop computer processing power.) One of the most common uses of chemometrics is the analysis of spectra generated from atomic absorption or atomic emission instrumentation, designed to predict the concentration of elements and compounds found in solid, liquid and gaseous materials. Since the LIBS process generates spectra similar to that of spectra induced by atomic absorption or emission analytical laboratory equipment, chemometric modeling is well suited for laser scanning. (The term multivariate chemometrics is technically redundant, but is used herein to assist in describing the nature of the models used to generate discriminatory or predictive outputs to evaluate laser-scanned aggregates.)

There is one major practical difference, however, between chemometrics used in the laboratory on small, typically homogeneous sample sets and laser scanning of heterogeneous aggregate materials analyzed under materials testing field conditions for which the SLT has been developed. To capture the nature of the material scanned, large quantities of data that must be collected and rapidly processed to convert the spectral output into useful engineering data. To achieve this end, part of the effort of NCHRP IDEA Project 168 focused on the development of the previously referenced specialized software, the SLTDAM software, to manage input and output data.

SLTDAM software incorporates chemometric models capable of communicating with the SLT system (i.e., the SLTOPS software) thereby providing a two-way communication between the laser scanning system (SLT) with such satellite systems (e.g., spectra in—engineering information out). Two related multivariate techniques are employed in the SLTDAM software: (1) Principal Component Analysis (PCA) and (2) Partial Least Squares Regression (PLS). A detailed description of these techniques is beyond the scope of this report but in general, PCA is used in the SLTDAM software as a discriminatory model to sort out dissimilar aggregate types from similar types, and PLS is used as a regression model to predict aggregate properties based on spectral emission data that has been calibrated to specific aggregate types and properties.

The main result of PCA is a PC score plot, which is a two-dimensional diagram that reduces the multidimensional nature of the analysis to a more familiar two-dimensional framework that can be visualized. The two dimensions of this plot represent a new coordinate system referred to as principal components (PC). The samples plot on this two-dimensional diagram can be interpreted like any two-dimensional (x vs. y) diagram. Samples that are similar in composition plot near each other and those with very different compositions will plot in a different section of the diagram. Two-dimensional plots (x vs. y) in univariate analyses define points in two-dimensional space. Samples that have similar x and y variables will plot close together, while samples with dissimilar variables will plot in different locations. A line (or vector) of best fit, oriented in the direction of maximum variance (least square regression line) can also be constructed through these points. In multivariate analyses there are more than two variables (~14,000 variables in this case). PC score plots depict multidimensional data in a pseudo-two-dimensional space, which is represented by principal components or eigenvectors. Eigenvectors are lines of maximum variance, similar to least square regression lines in two-dimensional space; however, they are oriented through variables plotted in multidimensional space and projected onto a two dimensional plane. Just as similar samples cluster in the same region of a two-dimensional plot, similar samples cluster in similar regions of a PC score plot. Samples that are similar in composition plot near each other and those with very different compositions will plot in a different section of the diagram.

PLS is similar to PCA but can be used to develop models that can project values (dependent variables) for unknown samples based on previously calibrated data generated from an original data set. The additional dependent variables can be values, such as specific gravity or acid insoluble residue. Like any calibration, once the model is calculated, one can input new spectra and calculate the values of the additional variable (this process is similar to linear regression analysis with two variables, where a calibrated data set is used as the basis for predicting dependent variables from unknown samples; but in this case the regression is occurring through multidimensional space, not two-dimensional space.) The additional variables can also be indicator integers. Integers “1” and “0” are used in aggregate analysis to model data in which there are yes or no questions that must be answered. For example, does the group contain a deleterious material or not (“Yes” being set equal to 1 and “No” being set equal to 0, or “belongs to group” being set equal to 1 and “belongs to some other group” being set equal to 0). The efficacy of PLS models are depicted by how well a predicted value correlates with a known input value. These are referred to as PLS validation plots.

Both PC score plots and PLS calibration and validation models are used to depict the results of the data analysis described in the next section of this report (during data analysis, commercially available multivariate statistical software (Unscrambler \circledR) was used as a check to ensure that SLTDAM could duplicate models generated by Unscrambler \circledR).

SCANNING RESULTS AND ANALYSIS

To evaluate the performance of the SLT prototype developed in this NCHRP 168 effort, aggregate samples were provided to the Research team from the states of Kansas, New York, Ohio, Oklahoma, and Pennsylvania for testing and evaluation. For each aggregate sample provided, test data on select aggregate properties were provided. A listing of samples and test data, provided by each respective state, is presented in Table 1.

Samples provided by each state for scanning were selected from a wide range of sources. A list of the types of samples received from each state and the samples' sources are summarized in Table 2. It is of note that the wide range of aggregate types and source locations, coupled with the relative small number of samples that were available

for scanning during this NCHRP 168 effort, were not ideal conditions for calibrating and validating aggregate chemometric models. Additional samples are needed. Nonetheless, as will be shown below, aggregate properties can be defined in most cases, suggesting that additional and more focused sample collection strategies would significantly improve the database [A wider sampling and scanning program is underway in a Transportation Pooled Fund Program: TPF 5(278)].

Each sample was contained within a 5 gallon bucket, containing approximately 3 to 4 gallons of aggregate material. Scanning was undertaken by routing the 3–4 gallon sample through the SLT and firing a total of 150 laser shots at the sample. The spectra associated with these 150 shots were averaged to yield one subsample spectra. This process was repeated ten times to yield 10 subsample spectral images, each representing the average of 150 laser shots. The 10 subsample results were further averaged to yield one super-averaged spectra to represent the one sample (in spectra averaging the intensity recorded at each wavelength is summed and divided by the number of laser shots).

TABLE 1
Summary of Number of Samples and Test Data Provided by States

Available Test Data	Kansas	New York	Ohio	Oklahoma	Pennsylvania	All States
AIR	36	16	—	8	—	60
Bulk Specific Gravity	36	—	14	33	14	97
SSD Specific Gravity	36	—	14	26	14	90
Apparent Specific Gravity	24	—	—	—	14	38
Absorption	36	—	14	33	14	97
Micro-Deval	—	—	—	27	14	41
LA Loss	36	—	8	33	14	91
Approved Materials	12	—	—	—	—	—
D-Cracking	35	—	—	—	—	—
% Chert	—	—	9	—	—	—
% Blast Furnace Slag	—	—	—	—	14	—

TABLE 2
Distribution of Sample Types and Sources from Five States

Source Description	Kansas ^a	New York ^b	Ohio ^c	Oklahoma ^d	Pennsylvania ^e
Limestone	x	x	x	x	
Gravel			x	x	
Sandstone				x	
Dolostone			x	x	
Blast Furnace Slag					x
Steel Slag					x
Recycled Concrete				x	

^aKansas samples were collected from at least seven different quarries around the state.

^bNew York samples were collected from three to four quarries.

^cOhio samples were collected from at least 15 different locations.

^dOklahoma samples were collected from at least 26 different locations and included quarry sites in Arkansas, Texas, and Colorado, as well as Oklahoma.

^ePennsylvania samples included blast furnace slag and steel slag blends collected from 14 different slag pile locations.

The efficacy of the modeled data was determined using one of two techniques: (1) test set validation and (2) cross validation. When a set of data is used to calibrate a model, the most effective approach is to obtain a set of samples

for use as a calibration set to calibrate the model, and then use a completely independent sample or validation set to validate the model. This method is referred to as “test set validation.” When there are an insufficient number of samples available to calibrate the model, in chemometric modeling the “cross validation” method is commonly used. In cross validation, the model is calibrated using all the data and then in a stepwise fashion one sample is removed from the model. A new calibration model is then generated without the left out sample. The sample left out is then used as a test sample. This process can be repeated until each sample in the model has been analyzed in this fashion. In general, in the NCHRP IDEA 168 effort there were an insufficient number of samples to use; however, wherever more than 20 samples were available, test set validation was attempted (although in some cases more than 20 samples were available, data associated with the property to be modeled was not).

Selected parameters were modeled from the available data from each state. The parameters modeled during this study are listed in Table 3.

TABLE 3
Modeled Test Data by State

State	Data Modeled
Kansas	Bulk Specific Gravity SSD Specific Gravity Apparent Specific Gravity D-Cracking Approved Materials Evaluation
New York	Friction (AIR)
Oklahoma	Absorption Micro-Deval Loss
Ohio	LA Loss Chert Content
Pennsylvania	Apparent Specific Gravity Micro-Deval Loss
Combined State Data	Bulk Specific Gravity Absorption

The following subsections summarize, by state, the procedures, results, and findings observed during the laser scanning and modeling efforts.

Kansas Testing

Samples received from Kansas DOT were scanned and modeled to evaluate how well the models could be calibrated to predict bulk specific gravity, saturated surface dry (SSD) specific gravity, apparent specific gravity, and D-cracking susceptibility. In addition, a special study was undertaken to assess whether pre-approved source materials introduced into a blend for concrete production could be identified in the final blended product. This special study is referred to in this report as the approved materials study.

Bulk, SSD, and Apparent Specific Gravity Results

PLS models were developed for bulk specific gravity, SSD specific gravity, and apparent specific gravity. The results, presented in Figures 6–9, are respectively presented in pairwise of figures depicting both the calibration and validation models developed using the scanned sample spectra. Figure 6 shows the results of the bulk specific gravity calibration model and Figure 7 the results of the bulk specific gravity cross validation model. PLS have a great deal of multi-dimensional data from which to develop effective calibrations. As a result, PLS models are expected to generate in most cases effective calibration models. This can be seen in the highly correlated calibration model presented in Figure 6 ($R^2 = 0.911$ and Line Slope = 0.911). A very good calibration correlation, however, need not translate into a very good validation model. In the validation model, sample data not included in the calibration model are used to test the model. This can be seen in the less than highly correlated validation model calibration model presented in Figure 7 ($R^2 = 0.396$ and Line Slope = 0.735911). Despite the reduced correlation in the validation model, these results clearly reveal that the models are recognizing the increasing sample specific gravity data trends. These results are impressive considering the wide geographic range covered by the samples collected from Kansas and the relatively small size of the sample set. Such results suggest that increasing the size of the sample set will improve both the calibration and validation models. An examination of the results for SSD yields similar pairwise calibration and validation models with highly calibrated models and correctly trending cross

validation models. The calibration and cross validation models for SSD specific gravity are respectively presented in Figure 8 and 9.

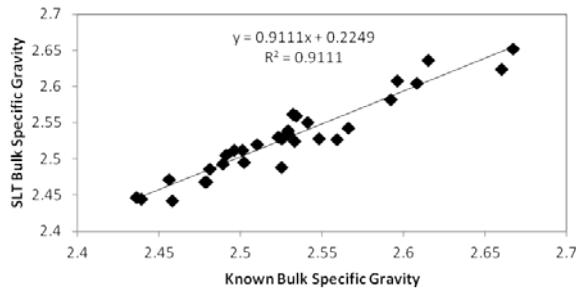


FIGURE 6 Kansas bulk specific gravity calibration model.

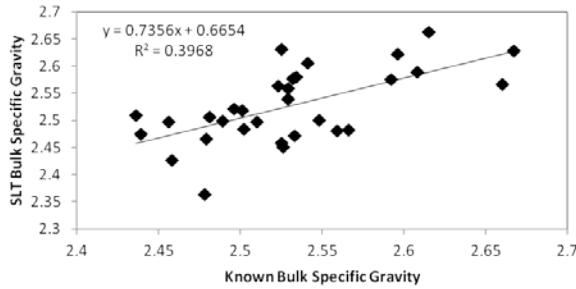


FIGURE 7 Kansas bulk specific gravity cross validation model.

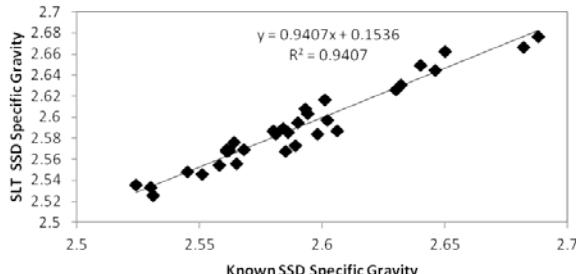


FIGURE 8 Kansas SSD specific gravity calibration model.

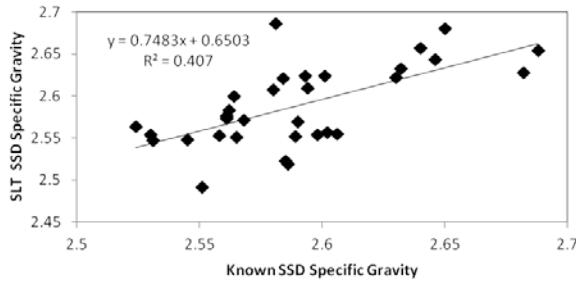
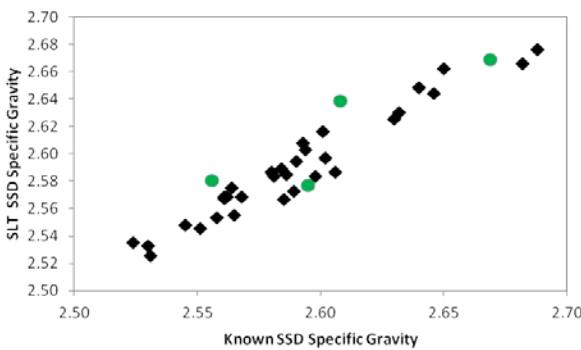


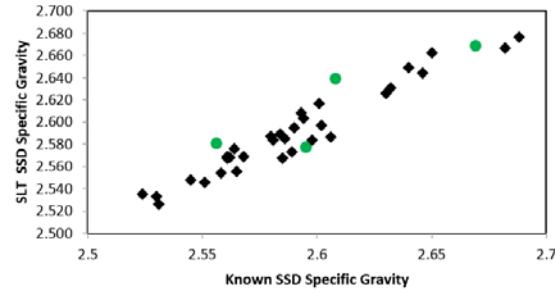
FIGURE 9 Kansas SSD specific gravity cross validation model.

Test set validation models were developed for the bulk, SSD, and apparent specific gravity models. A total of 36 samples were available for model development. Four KS samples were left out of the three calibration models; and each of the three models were calibrated with the remaining 32 samples. The four samples were then inserted into each model to predict the bulk, SSD, and apparent specific gravity values. Test set validation results are presented in Figures 10, 11, and 12, respectively. Each figure shows the calibration results (diamonds) and the test set validation results (circles). The actual values and the respective errors between the measured and predicted are included in tabular form in each figure. Each test set yielded impressive predictive results. Bulk specific gravity (BSG) and saturated surface dry (SSD) specific gravity prediction results were unexpected. It was assumed that apparent (true) specific gravity (ASG) would be most directly related to the spectral fingerprint, which would reflect the unique chemical makeup of the aggregate material. Bulk and SSD, however, introduce void space and moisture, respectively into the specific gravity calculation. The spectral signal does not directly measure void space or water saturated permeable voids. It is believed that the bulk and SSD specific gravity observation are due to a nearly-constant numerical shift in the regressed values used in the calibration models, where $BSG = C_1 \times (ASG)$; and $SSD = C_2 \times (ASG)$, and $C_1 < C_2$. As a result, once the ASG spectra are determined, the known BSG and SSD values used in the regression automatically make the C_1 and C_2 corrections.



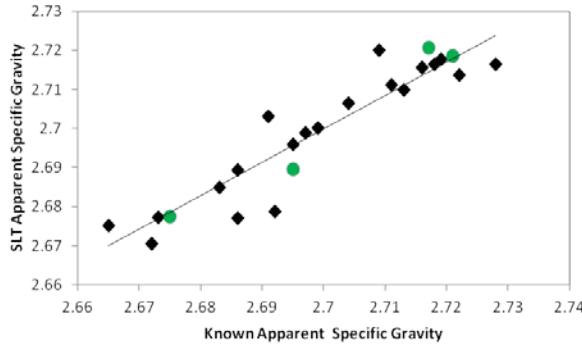
KS SSD SG Test Set				
	predicted	deviation	known	abs error
KS09	2.67	0.02	2.67	0.00
KS19	2.58	0.03	2.60	0.02
KS23	2.58	0.04	2.56	-0.03
KS30	2.64	0.03	2.61	-0.03

FIGURE 10 Kansas bulk specific gravity test set calibration and validation.



KS SSD SG Test Set				
	predicted*	known	abs error	% error
KS09	2.669	2.669	0.000	0.00
KS19	2.577	2.595	0.018	0.68
KS23	2.581	2.556	-0.025	-0.97
KS30	2.639	2.608	-0.031	-1.18

FIGURE 11 Kansas SSD specific gravity test set calibration and validation.



KS Apparent SG Test Set				
	predicted	deviation	known	abs error
KS09	2.72	0.03	2.72	0.00
KS19	2.72	0.05	2.72	0.00
KS23	2.68	0.03	2.68	0.00
KS30	2.69	0.04	2.70	0.01

FIGURE 12 Kansas apparent specific gravity test set calibration and validation.

D-Cracking Results

A total of 35 samples (designated KS1-KS35) were used in the Kansas D-cracking studies. The goal in this study was to separate samples into two groups: those that would pass the D-cracking test and those that would fail. PLS models were generated, using the integer regression variable “1” for passing samples and the integer regression variable “0” for failing samples. Once a model was calibrated by setting passing and failing samples to these values, the predicted variable was calculated for a selected set of test set samples. Samples with calculated variables closer to 1 were assigned to the passing group; those with calculated variable closer to 0 were assigned to the failing group. A value called the VAD (Value of Apparent Distinction) was used to separate the two groups. The VAD is chosen

during calibration to give the best fit to the model.

The D-cracking pass/fail model was calculated twice, with two different sets of test set samples. Figure 13 shows the results of the calibration for the first model, in which passing samples KS-22 and KS-41 and failing samples KS-9 and KS-43 were reserved for test set validation. Using a VAD of 0.4, the calibration was 90% successful; only three samples were misclassified. The exercise was repeated using four different samples for test set validation (passing samples KS-29 and KS-11, failing samples KS-8 and KS-37). The results of the calibration are shown in Figure 14. Again, the model was 90% successful, with a VAD of 0.4, and only misidentifies three samples.

The test set samples KS-9, 22, 41, and 43 were run through the model and the predicted variable values were determined. The results, listed in Table 4, show that the model correctly predicted whether all four samples would pass or fail. For the test set samples KS-29, KS-11, KS-8 and KS-37, three of the four test set samples were correctly identified. Sample KS-37 had a calculated value of 0.81, above the VAD of 0.4, and so would be assigned to the group of passing samples, although it is a failing sample. Overall, seven of eight samples were correctly identified, for a success rate of 87.5%.

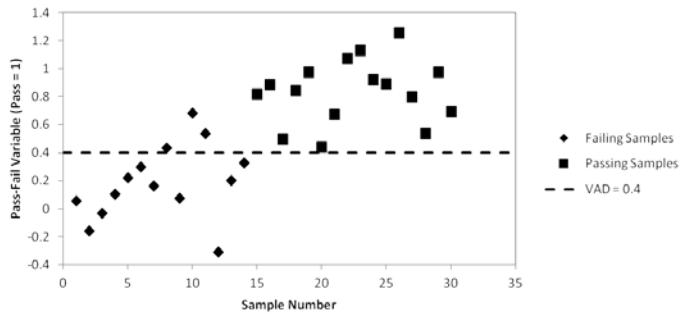


FIGURE 13 Kansas calibration results for first D-cracking pass-fail model (90% success rate).

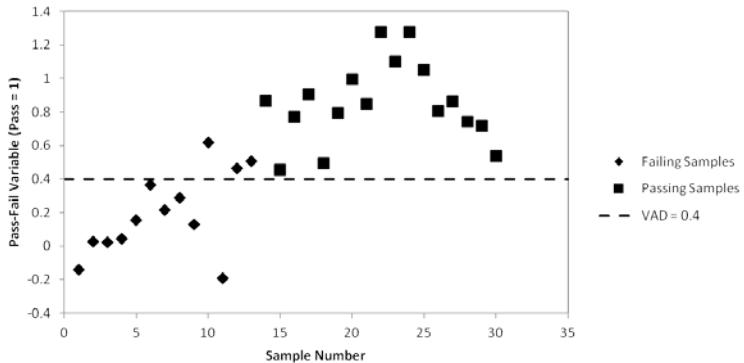


FIGURE 14 Kansas calibration results for second D-cracking pass-fail model (90% success rate).

TABLE 4
Results of D-cracking Pass-Fail Models with KSDOT Samples

Sample	Known to Pass or Fail	Calculated Variable	Correct?
KS-9	Fail	0.21	yes
KS-43	Fail	0.24	yes
KS-22	Pass	0.97	yes
KS-41	Pass	0.45	yes
KS-8	Fail	-0.36	yes
KS-37	Fail	0.81	no
KS-29	Pass	0.49	yes
KS-11	Pass	0.65	yes

Approved Materials Evaluation

KSDOT submitted a special set of aggregate samples for laser scanning to determine whether the set of materials used in a production (blending) process located at a quarry site consisted of aggregate from pre-approved material beds or perhaps non-approved materials. The samples submitted for testing, listed in Table 5, show that beds KS-34 and KS-35 were D-cracking approved samples, but samples KS-32 and KS-33 were not. Production samples KS-41 through KS-47 were approved as mixtures of KS-34 and KS-35, but failed KSDOT D-cracking specifications. The questions raised were as follows:

- Are samples KS-41 through KS-47 blends of KS-34 and KS-35?
- Are they blends that use KS-32 or KS-33?
- Are they blends of some other aggregate?

TABLE 5
Samples Used in KSDOT
Approved Materials Study

Sample	Status
KS-32	Not approved
KS-33	Not approved
KS-34	Approved
KS-35	Approved
KS-41	??
KS-42	??
KS-43	??
KS-44	??
KS-45	??
KS-46	??
KS-47	??

This problem was approached using Principal Component Analysis. Figure 15 shows a PC score plot of the samples. On score plots, as previously noted, samples that are similar in composition plot near each other, and samples that are different plot far from each other. Blends of two samples fall along a straight line between the two end-members. KS-34 and KS-35 plot near each other in the lower right corner of the diagram; KS-32 and KS-33 are clearly not similar to KS-34 and KS-35. More importantly, the production samples (black squares, representing KS-41 to KS-47) do not plot as a straight line between approved beds KS-34 and KS-35. Neither do they appear to be blends of any of the four beds. The production samples do, however, define a straight line between either KS-33 or KS-32 and some other sample that was not analyzed in this study but whose composition lies beyond the lower left side of the diagram. These data suggest that

- Samples KS-41 through KS-47 are not blends of KS-34 and KS-35.
- Samples KS-41 through KS-47 are not blends of KS-32 or KS-33.
- Samples KS-41 through KS-47 are possibly blends of KS-33 with some other material not provided.

This exercise illustrates that the SLT can be used to rapidly detect variations in production samples. These samples all look very similar; there was no reason to exclude them from use until they started to fail D-cracking tests. SLT analysis would detect non-approved material use in production blends in near real time.

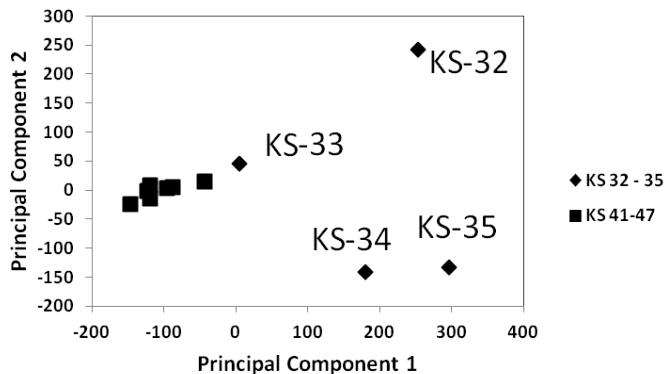


FIGURE 15 Kansas score plot: Approved materials study, New York Testing.

Acid Insoluble Residue Testing

One parameter was modeled with New York aggregates: Acid Insoluble Residue (AIR). A list of the aggregates prepared and scanned for AIR analysis is presented in Table 6. Five separate aggregates supplied by NYSDOT and a set of 11 blends created from two of the aggregates were analyzed. The blends were created by mixing Becraft (11.9% AIR) and New Scotland (54.9% AIR).

TABLE 6
Measured AIR Values for NYSDOT Samples

Sample Name	AIR %	% Becraft/ % New Scotland
NY-B0	54.9	100/0
NY-B10	52.23	90/10
NY-B20	44.40	80/20
NY-B30	39.40	70/30
NY-B40	31.60	60/40
NY-B50	34.10	50/50
NY-B60	29.40	40/60
NY-B70	24.63	30/70
NY-B80	19.60	20/80
NY-B90	14.00	10/90
NY-B100	11.90	0/100
1.2RDriedScreening	32.70	
100 Becraft	11.90	
100 New Scotland	54.90	
E Kingston	53.60	
LabBlend	29.10	

Test set modeling was used to determine the accuracy of predicting AIR using SLT data. Two test set models were created. The first model removed samples 1.2RDriedScreening and 100 Becraft from the calibration and then used the model to predict AIR in these two samples. Figure 16 shows the calibration results (diamonds) and the test set validation results (circles).

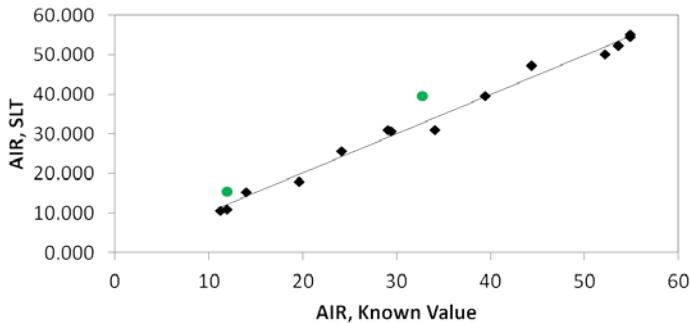


FIGURE 16 NY AIR Test Set Validation (1) calibration (diamonds) and test set validation (circles).

The calibration model is very good with an r^2 value equal to 0.989. Test set validation samples modeled relatively close to the known values. The 1.2RDriedScreening, with known AIR of 32.7% was analyzed at 39.6%, and 100 Becroft with known AIR of 11.9% was analyzed at 15.5%.

The second test set model was created using samples East Kingston and LabBlend as the test set validation samples. Results are shown in Figure 17. The second calibration was also excellent with an r^2 value of 0.966. East Kingston (known AIR = 53.6%) was modeled at 36.2%, and sample LabBlend (known AIR = 29.1%) was modeled at 21.5%.

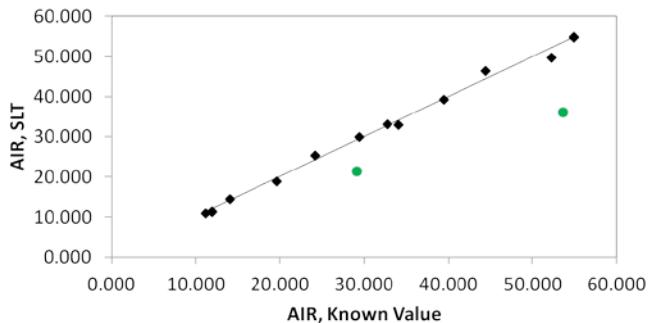


FIGURE 17 NY AIR Test Set Validation (2) calibration (diamonds) and test set validation (circles).

While these results indicate that the SLT data can be modeled to estimate AIR values, the results are not yet as accurate as desired. One reason for this is that the majority of the calibration curve in these models is from samples blended from the Becroft and New Scotland samples; that is, the calibration is controlled almost entirely by the compositions of two aggregates. If a larger number of aggregates with known AIR values were used to calibrate, it is projected that the predictions would be more accurate.

Ohio Testing

Scanned Ohio samples were modeled for LA Loss and chert content.

LA Loss Testing

It was originally assumed that since LA Loss is a measure of degradation by abrasion, impact, and grinding, correlating chemically dominant spectral data with LA Loss would not be very productive. The project team's attempts at modeling LA Loss with ODOT samples, however, suggest that it might be possible to model LA Loss.

Ohio submitted eight samples with LA Loss measurements, which is too few to calculate a model with confidence. The calibration of these data is presented in Figure 18. The calibration was very good, however, with $r^2 = 0.984$ and a slope near 1. Validation of the calibration was performed with cross validation. The results, shown in Figure 19, are not as good; however, the LA Loss cross validation results are trending in the right direction with a moderately good correlation, suggesting that this model has promise if a sufficient number of samples are used. In cross validation, one sample is left out of the calibration so that its value can be calculated. With only eight samples, each sample is very important to the calibration, and the model suffers when only seven samples are used.

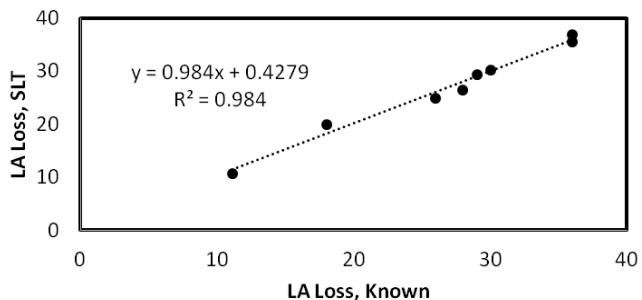


FIGURE 18 Ohio sample calibration model for LA Loss.

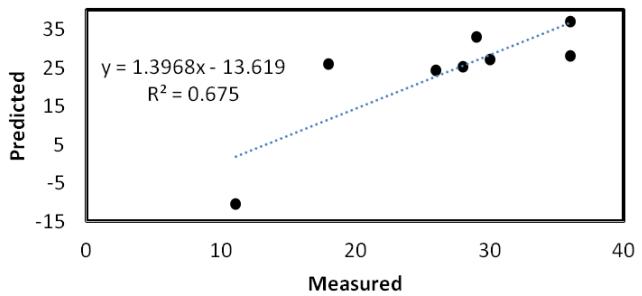


FIGURE 19 Ohio cross validation model for LA Loss.

Chert Content

Nine samples received from Ohio DOT were used to develop a chert content model. The calibration model for chert content is shown in Figure 20; the cross validation model is shown in Figure 21. The calibration is fairly good, with high r^2 and slope near 1, although the slope is strongly controlled by the one sample with more than 10% chert. As with the LA Loss model, cross validation results do not correlate nearly as well as the calibration model; however, the results trend in the right direction, suggesting that the data should be improved with a larger sample set.

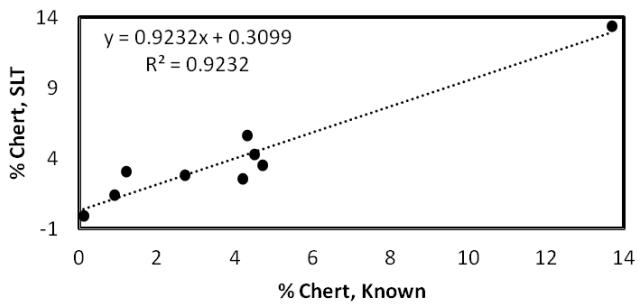


FIGURE 20 Ohio calibration model for chert content.

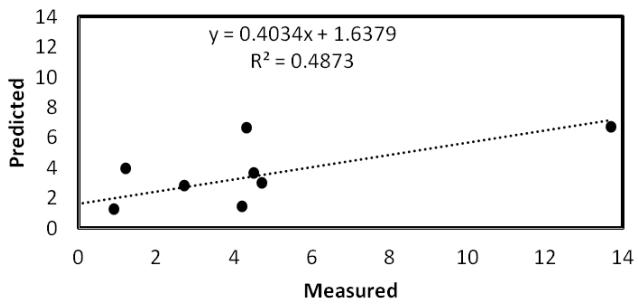


FIGURE 21 Ohio cross validation model for Chert Content.

Oklahoma

Samples received from Oklahoma had significant lithological and geographic diversity. Supplied samples, as listed in Table 2, were from Oklahoma, Texas, Arkansas, and Colorado. They consisted of limestones, various gravels, sandstones, and recycled concrete aggregate. Although there are 33 samples, the diversity of the sample set needs even more samples to completely represent all the different compositions. Oklahoma aggregates were modeled for absorption and Micro-Deval Loss.

Absorption Testing

A total of 33 Oklahoma samples were available for absorption analysis. Of the 33 Oklahoma samples analyzed, four samples were found to be significant outliers and were removed from the model. The calibration for the Oklahoma absorption model is presented in Figure 22. There is significant scatter, but the trend is in the right direction. Results for four test set samples are plotted in Figure 23. Again, the results are not yet ideal, but given the wide range of sample variability the results are encouraging and suggest that improvements in sample selection would yield improved results.

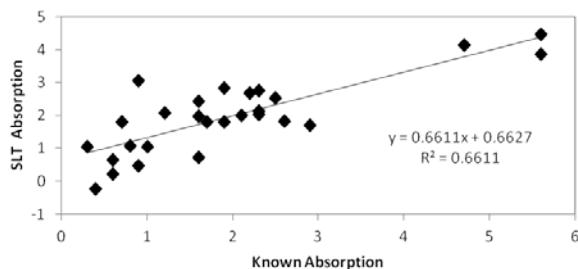


FIGURE 22 Oklahoma calibration model for absorption (four outliers removed).

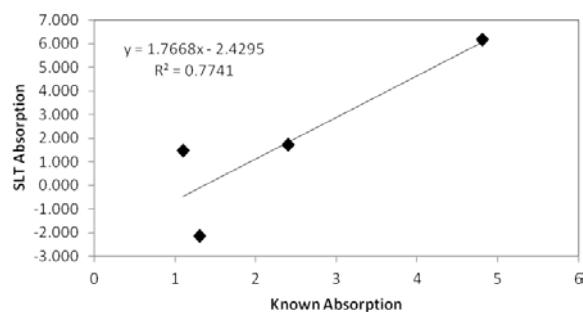


FIGURE 23 Oklahoma test set validation model for absorption (four outliers removed).

Micro-Deval Loss Results

The calibration for the Micro-Deval model is presented as Figure 24; the cross-validation results are presented in Figure 25. Due to the heterogeneity of the Oklahoma sample set, only limestone scans were included in the model calibration and validation process.

The calibration model developed exhibited very high correlation. As previously noted, multivariate chemometric models have the capability to generate highly correlated calibration models, but this does not necessarily translate into effective predictive models. If the spectral information used to develop the calibration model does not contain sufficient information to define the spectra associated with the samples being tested, then the validation results will not be good. The cross-validation results presented in Figure 25 are poorly correlated. It is noteworthy, however, that the cross validation regression line tracks the calibration model trend quite well. This type of graphical results suggests that the model on average sees the correct trend, but additional calibration data (samples) are needed to provide the information necessary to define the wide heterogeneity associated with the Oklahoma sample set.

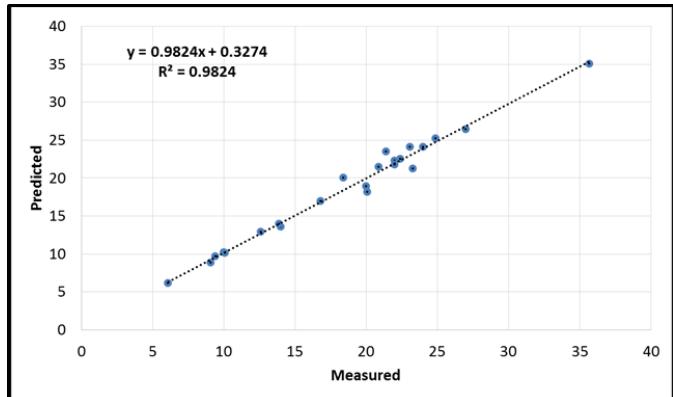


FIGURE 24 Oklahoma calibration model for Micro-Deval Loss (outliers removed).

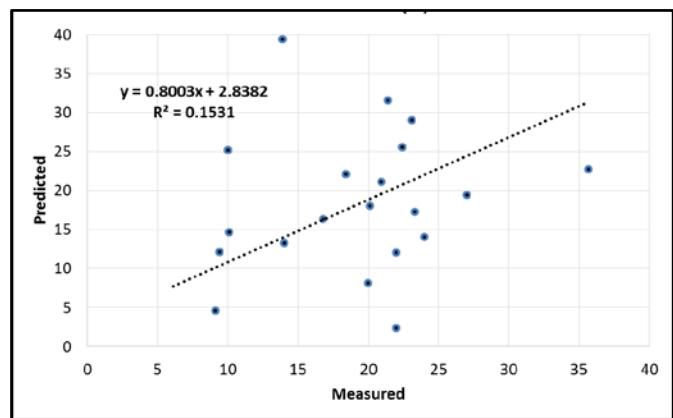


FIGURE 25 Oklahoma cross validation model for Micro-Deval Loss (outliers removed).

Pennsylvania

PADOT submitted 14 mixed slag samples collected from 14 different slag piles for testing. Scanned spectra were modeled for apparent specific gravity and Micro-Deval Loss.

Apparent Specific Gravity Results

The calibration and cross validation model results for apparent specific gravity are presented in Figures 26 and 27, respectively. Given the small sample set and the slag variability encountered, the validation results, while not highly accurate, provide a clear positive trend.

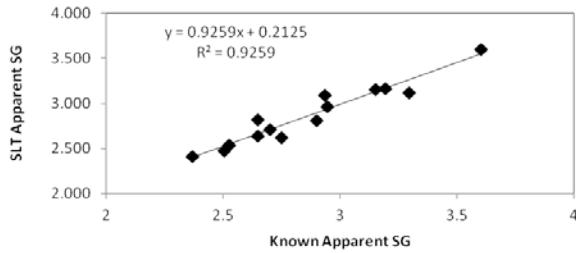


FIGURE 26 PA calibration model for Apparent Specific Gravity.

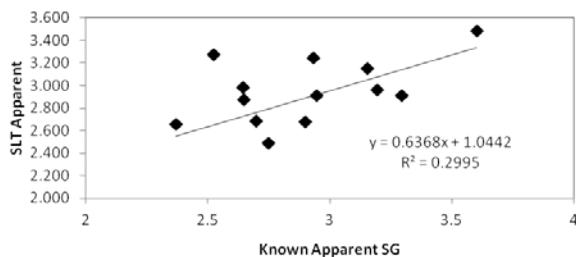


FIGURE 27 PA cross validation model for Apparent Specific Gravity.

Micro-Deval Loss Results

The calibration for the Micro-Deval model is presented as Figure 28; the cross-validation results are presented in Figure 29. The calibration is strong, with highly correlated results. The cross-validation results are less well correlated with known composition, but are clearly tending in the correct direction.

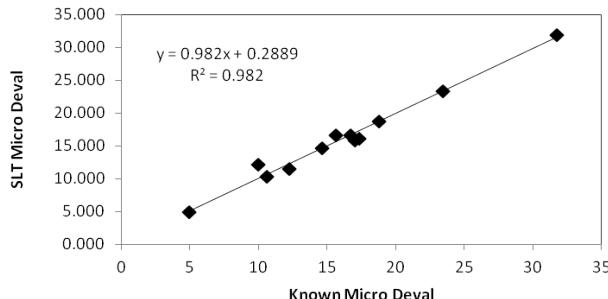


FIGURE 28 PA calibration model for Micro-Deval.

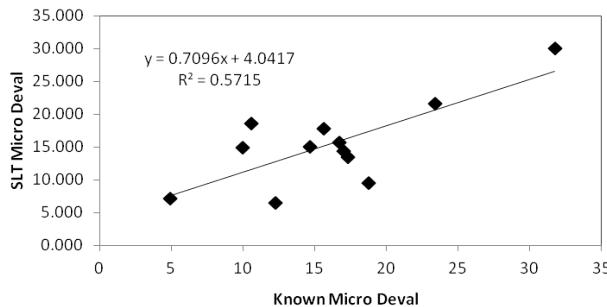


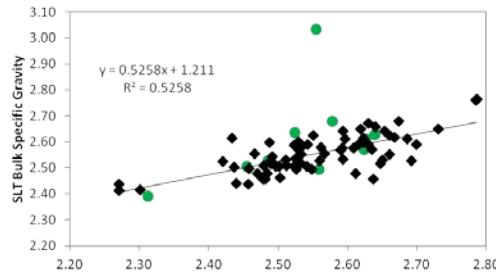
FIGURE 29 PA cross validation model for Micro-Deval.

Combined State Data Analysis

While work to date has revealed that modeling of SLT spectra is much improved with a larger number of samples, a large variability in the type of samples may in and of itself require additional samples to address the wide range of heterogeneity associated with aggregate samples. Nonetheless, modeling was undertaken with spectra from all of the states combined to create mega-models where data were available (i.e., data were supplied by the participating states). In this section, modeling of bulk specific gravity is presented.

Bulk Specific Gravity Results

The largest quantity of data available was bulk and SSD specific gravity data. All states, with the exception of New York, reported bulk specific gravity and SSD specific gravity results on all samples. The bulk specific gravity model calibration and test set validation results for the combined Kansas, Oklahoma, and Ohio data are presented in Figure 30. The results of the test samples, presented in the table below the calibration model, shows most test samples to be within ± 0.06 of known values.



	predicted	deviation	known	abs. error
KS9	2.63	0.07	2.64	0.01
KS19	2.64	0.05	2.52	0.02
KS23	2.53	0.08	2.49	-0.06
KS30	2.50	0.08	2.56	-0.03
OH1	2.68	0.10	2.58	0.18
OH8	2.57	0.06	2.62	0.08
OK12	2.61	0.12	2.63	0.01
OK18	3.03	0.62	2.55	0.50
OK23	2.39	0.07	2.31	-0.12
OK32	2.51	0.13	2.45	-0.03

FIGURE 30 Combined states (Kansas, Oklahoma, and Ohio) Bulk Specific Gravity Calibration and Test Set Validation.

The models for SSD specific gravity using samples are shown in Figure 31. The calibration shows a slope nearer 1 and a higher correlation coefficient. Test set results are also better for SSD specific gravity than for bulk specific gravity, with absolute errors generally less than 0.9.

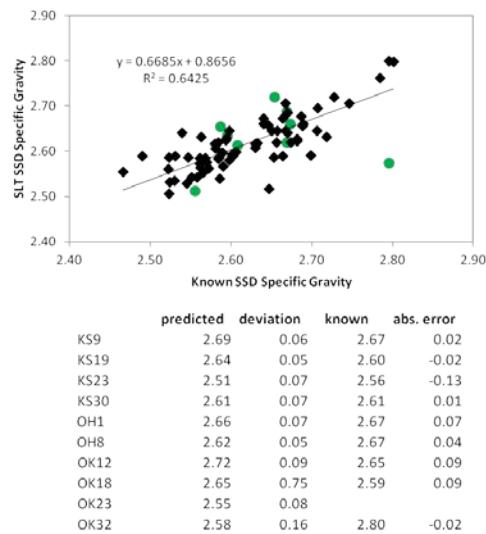


FIGURE 31 Combined states (Kansas, Oklahoma, and Ohio) SSD Specific Gravity Calibration and Test Set Validation.

Absorption Results

The combined modeled results for absorption are shown in Figure 32. Aggregates from Kansas, Ohio, Oklahoma, and Pennsylvania were used in the model; test set samples were chosen from Kansas, Ohio, and Oklahoma. Instead of modeling the actual absorption value for an aggregate, samples were separated into two groups: greater than or equal to 2.5% absorption and less than 2.5% absorption (this VAD model was selected after attempts to model actual absorption values proved unsuccessful). Here, the calculated absorption variable (1, if absorption is greater than or equal to 2.5%; and 0, if absorption is less than 2.5%) for calibration samples is plotted against sample number. Four samples are misidentified, using a VAD of 0.4, yielding an overall success rate of 95%. The results of test set validation for ten samples are also presented in tabular form in Figure 32. Nine of the ten samples are correctly assigned to the correct group using the VAD = 0.4 chosen during calibration. The model was 90% successful in predicting whether an aggregate has greater than 2.5% absorption or less than that threshold value.

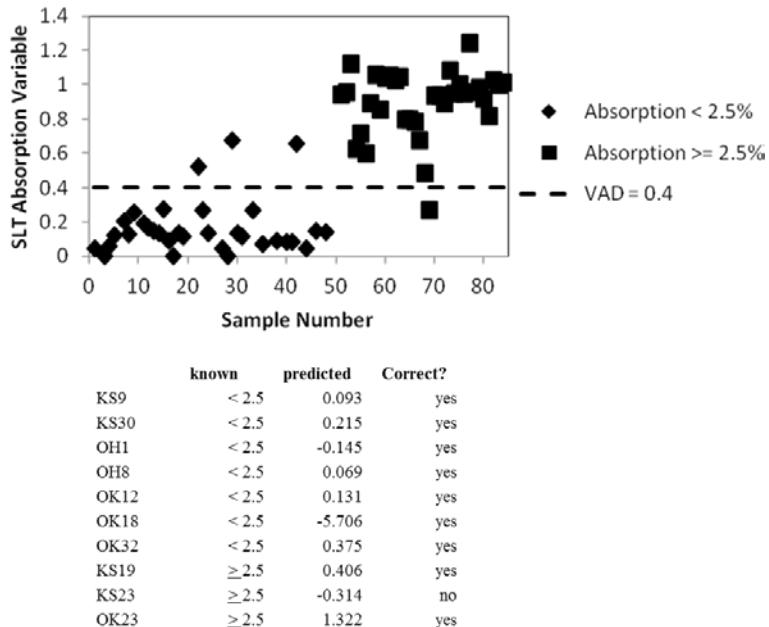


FIGURE 32 Combined states (Kansas, Ohio, and Oklahoma) VAD Model for Absorption.

FINDINGS AND CONCLUSIONS

NCHRP IDEA Project 168 effort focused on the development of laser scanning equipment that could be used to provide a tool for real time scanning of aggregate materials for quality control (QC). As part of this effort a system referred to as the Sampling Laser and Targeting System (SLT) was designed, fabricated and tested to assess how well the prototype could perform as a rapid scanning tool.

Technical research findings were as follows:

- The SLT prototype system developed during the course of this study was capable of routine analysis of approximately 8 to 12 aggregate samples on a daily basis, and capable of scanning bulk aggregate samples in near real time.
- Emission spectra recorded (at wavelengths ranging from 200 nanometers (nm) to approximately 980 nm, derived from averaging spectra generated by firing 1,500 individual laser shots from a high-powered, pulsed Nd:YAG laser at aggregate samples), provided the means to generate data that could discriminate among aggregate samples tested in this research effort.
- Multivariate (chemometric) calibration models and validation tests on these models, developed to predict values for AIR, bulk specific gravity, SSD specific gravity, apparent specific gravity, absorption, Micro-Deval, approved materials, D-cracking, and percent chert, yielded very promising results.
- The efficacy of such models is dependent on the calibration procedures employed in the process and in particular the heterogeneity of the aggregate test sample set.
- This heterogeneity of aggregate samples provides a great deal of information that must be incorporated into chemometric models to provide the information necessary to develop accurate predictive models.
- The relatively small number of samples tested to date and the large variability in the types of samples tested, limited the accuracy of the validation test predictions during this investigation.
- Additional software improvements that provide intensity normalization and drift corrections procedures as well as spectral outlier detection will improve modeling resolution.

It was concluded from these findings that

- Laser scanning in near real-time of aggregate materials is a technology capable of significantly improving the manner in which aggregate quality control procedures are employed by the industry, altering the paradigm of aggregate monitoring established in the early 20th century.
- The SLT prototype developed during the course of this investigation provides a system capable of processing aggregate samples and can be operated by material technicians with no special training,
- The development of the technology will require establishing suitable and expanded laser-induced spectral information databases for target aggregates of interest, with sufficient numbers and types of sample to properly characterize the target property.
- Improvements in data analytical techniques still being evaluated will further assist in resolving the spectral information generated during the laser scanning process and improving model predictions of aggregate properties.

PLANS FOR IMPLEMENTATION

The SLT Research Team is proceeding with the development of this technology. Future implementation plans are divided into near- and longer-term objectives. Near-term objectives represent plans extending approximately 12–18 months into the future. Longer-term objectives represent activities beyond this 18 month near-term period.

Near-Term Objectives

The near-term objectives are intended to further establish the system performance capabilities and to upgrade the SLT prototype (hardware and software) to the next generation system; and to further develop public and private sector participation in the technology.

Development of this technology and its commercial application in the materials and highway sector as a rapid scanning QC tool is heavily dependent on both public and private sector support and acceptance of the technology. In particular, since aggregate quality is defined almost exclusively by public sector specifications and test procedures, it is imperative that the public sector play a major role in this developmental process. This will require multi-state and where possible federal support and promotion.

As previously discussed, a Transportation Pooled Fund Study (TPF 5[278]), which includes the participation of five states (Kansas, Oklahoma, Ohio, New York, and Pennsylvania), is ongoing and is expected to yield much more data on the system. Samples are being collected for additional testing from private sector companies as well as state agencies.

Longer-Term Objectives

In the longer term, to transition from a testing evaluation process to a commercial system, additional SLT systems will need fabrication. Deployment will be necessary at multiple public and private facilities around the nation. The development of centralized (repository) databases will be required; and local regional and nationwide databases established. During the near term, plans will be implemented to initiate this long-term strategy.

REFERENCE

Chesner, W.H. and N.J. McMillan, *Automated Laser Spectrographic Pattern Matching for Aggregate Identification*, Final Report for Highway IDEA Project 150, Transportation Research Board of the National Academies, Washington, D.C., April 18, 2012.

APPENDIX A

Draft Standard Recommended Practice for Rapid Classification of the Type and Engineering Material Properties of Highway Aggregates Using Laser Scanning and Multivariate Modeling

Draft Standard Recommended Practice for

Rapid Classification of the Type and Engineering Material Properties of Highway Aggregates Using Laser Scanning and Multivariate Modeling

AASHTO Designation: PP _____

1. SCOPE

- 1.1 This practice covers the use of an aggregate laser scanning system that can be used to discriminate between aggregate types and to provide a means to predict the engineering properties of the aggregate scanned in near real time.
- 1.2 The practice includes a description of the significance of this technology to the highway industry, how the technology works, how mathematical models are employed to process the scanned data, the type of equipment used to scan the target material, personnel needs and their required level of expertise.
- 1.3 An expanded terminology section is provided to clarify terms used in this practice that are not common to the highway design and construction industry.
- 1.4 *This standard describes a system that employs a high-powered Class IV laser. Class IV lasers are a hazard to the eye from the direct beam and specular reflections and sometimes even from diffuse reflections. Class IV lasers can also start fires and can damage skin. Class IV lasers do not pose any radioactive threat. Equipment employed in this practice must be adequately constructed in accordance with appropriate safety regulations. Operating and maintenance personnel must be adequately trained in the preventive measures, such as appropriate eyewear and laser interlock mechanisms to be used when operating or maintaining the equipment.*

2. REFERENCED DOCUMENTS

2.1 AASHTO Standards:

- T 2-91 (2010), Sampling of Aggregates
- T 248-14, Reducing Samples of Aggregate to Testing Size

2.2 ASTM Standards:

- E2617-10, Standard Practice for Validation of Empirically derived Multivariate Calibrations
- E1655-05 (Reapproved 2012), Standard Practices for Infrared Multivariate Quantitative Analysis
- E122-09e1, Standard Practice for Calculating Sample Size to Estimate, With a Specified Tolerable Error, the Average for a Characteristic of a Lot or Process

2.3 NCHRP Reports:

- NCHRP Highway IDEA Project 168, Prototype Development: Automated and Continuous Aggregate Sampling and Laser Targeting System, 2015

3. TERMINOLOGY

- 3.1 Aggregate quality refers to a classification of the suitability of an aggregate for use in a particular highway application determined by its physical, chemical or mechanical properties as defined by existing AASHTO, ASTM, or Transportation Agency criteria specifications.
- 3.2 Aggregate source refers to a unique quarry, quarry ledge, gravel pit, stockpile or a distinct unit from which the aggregate was derived that exhibits unique properties (see Property).
- 3.3 Atomic emission spectroscopy is a method of chemical analysis in which a high energy thermal environment induced, for example, by an electric arc, a flame, or an inductively coupled or laser-induced plasma raises the energy level of atoms to excited states (see energy levels). This excitation results in a spontaneous emission of electromagnetic radiation that can be detected as a light spectrum with unique wavelengths and intensities.
Discussion- The wavelengths and intensities are characteristic of the element(s) and the elemental concentrations comprising the sample tested. The observed wavelengths and intensities are sometimes referred to as spectral or emission lines. The wavelength of the atomic spectral line gives the identity of the element while the intensity of the emitted light is proportional to the number of atoms of the element.
- 3.4 Chemometrics is a term used to describe the performance of calculations on measurements of chemical data or spectra derived from chemical data.
Discussion- In this practice, chemometrics refers to the art of performing calculations to convert spectral data generated by laser-induced spectral lines derived from an aggregate sample into variables that can assist in defining aggregate quality or material engineering properties.
- 3.5 Chemometric modeling refers to the application of chemometrics (see definition above) using multivariate modeling methods.
Discussion - In this application chemometric modeling refers primarily to principal components analysis and partial least squares regression analysis to generate models that can be used to discriminate between aggregate type, qualities and material sources; and correlate aggregate quality or engineering material properties with the spectral lines detected during the laser scanning process.
- 3.6 Compositional models refer to chemometric models that can predict a numeric value usually in the form of a percentage that relates to an engineering material property (e.g., LA loss, Micro-Deval loss, acid insoluble residue, percent chert).
- 3.7 Data analyst refers in this practice to the person that develops the chemometric models and analyzes the spectral emission data generated during the laser scanning process, yielding the chemometric model output.
- 3.8 Discriminant analysis is a form of modeling that permits a data analyst to classify two or more groups or clusters or populations when the characteristics of these groups are known.
Discussion – In discriminant analysis, once a calibration model is developed that can distinguish between classes of aggregate, one or more new observations can then be classified into one of the known groups based on the similarity or closeness of the new observation to each of the classified groups. As a simplified example, if two separate groups can be characterized as passing (P) and failing (F) aggregates for a specified test method a new observation or unknown aggregate could be analyzed to determine which of the groups the unknown aggregate is most similar to (i.e., the P group or the F group).
- 3.9 Electromagnetic radiation (EMR) consists of electromagnetic waves that travel at the speed of light in a vacuum, and include gamma rays, x-rays, ultraviolet, visible light, infrared, and radio waves that can be expressed in terms of energy, frequency or wavelength.

Discussion - In this practice, EMR primarily refers to the radiation emitted from the aggregate during the LIBS process (see Laser-induced breakdown spectroscopy) and is generally found to be in the range of approximately 200 to 1000 nanometers.

- 3.10 Energy level(s) is a term used to describe the degree of excitation of electrons in atoms, ions, or molecules that are bound by the electric field of the nucleus, and is a measure of their specific energy values (quantum number). If an atom, ion, or molecule is at the lowest possible energy level, it and its electrons are said to be in the ground state. If it is at a higher energy level, it is said to be excited.

- 3.11 Engineering material property refers to a property (see property) of an aggregate defined by test methods prescribed by AASHTO, ASTM, or Transportation Agencies that describe a unique characteristic that helps to assess the suitability of the aggregate for use in a particular highway application.

Discussion—Typical engineering material properties include specific gravity, absorption, organic content, abrasion resistance, hardness, soundness, freeze thaw resistance, friable particles, insoluble residue, aggregate reactivity (e.g., alkali silica reactivity, alkali carbonate reactivity D-cracking).

- 3.12 A laser is a device that projects a highly concentrated (collimated) narrow beam of light (or electromagnetic radiation) at nearly one specific wavelength (monochromatic), in which all the light waves travel in tandem (coherent).

Discussion—In this practice the narrow beam of light generated by a laser is further focused with lenses and pulsed to produce a small point of intense power to ablate a small portion of aggregate material during the laser scanning process.

- 3.13 Laser-induced breakdown spectroscopy (LIBS) is a type of atomic emission spectroscopy which uses a highly energetic laser pulse as the excitation source.

- 3.14 Maintenance engineer refers in this practice to the engineer or technician responsible for maintaining the operation of the laser scanning system.

- 3.15 Multivariate analysis comprises a set of statistical techniques dedicated to the analysis of data sets with more than one variable.

Discussion—When the variables examined are chemical data or chemical induced spectra the term chemometric analysis or chemometrics is commonly used interchangeably with multivariate analysis.

- 3.16 Model accuracy is a measure of the proximity of the predicted model value to the true value of the sample.

Discussion—There are numerous methods that can be employed to make this assessment. For example when subjected to discriminant analysis modeling with a binary output such as pass-fail or yes-no, the accuracy can be expressed in terms of percent correct predictions. If a compositional model is employed to provide a quantitative prediction of a specific property absolute or relative error can be used. A more detailed description of recommended statistical options is presented in ASTM 2617.

- 3.17 Partial least squares (PLS) regression analysis is a multivariate statistical technique that simultaneously correlates multiple independent variables to a dependent variable.

Discussion—In the context of this practice PLS is used to correlate the spectral patterns (wavelengths and intensities) induced by the LIBS process, which represent the independent variables to a defined variable (e.g., classification or property).

- 3.18 Pattern matching, sometimes referred to as pattern recognition, refers to the “learning” of multivariate models to identify and differentiate between spectral lines or wavelength patterns between and among sample types.

- 3.19 Principal components analysis (PCA) is a multivariate statistical technique that simultaneously analyzes multiple variables associated with a series of objects to compare similarity and differences between objects, simultaneously providing information on the contribution of each variable to the observed similarities or differences.
- Discussion*—In the context of this practice the multiple variables are represented by the spectral wavelengths; and the values of each variable is represented by the wavelength intensity.
- 3.20 Property is a material trait that defines quantitatively or qualitatively the response of a material to external stimuli when placed in a specific environment.
- Discussion*—Material scientists in general group material properties into six categories including mechanical, electrical, thermal, magnetic, optical and deteriorative (or chemical reactivity). Highway engineers tend to focus on mechanical and deteriorative properties. (see engineering material property).
- 3.21 Real time refers to the processing of information in a short period of time on the order of seconds or minutes to yield an answer regarding the desired aggregate characteristic.
- 3.22 Sampling and laser targeting system (SLT) refers to an existing laser scanning system currently employed to scan and determine aggregate quality (see NCHRP 168 for a detailed description of the system).
- 3.23 Spectral lines or patterns are the resulting emission lines (see atomic emission spectroscopy) observed when electrons transition from high energy levels to lower energy levels.
- Discussion*—Each element has a unique set (number and arrangement) of electrons and the energy differences between the electron orbits. This is due to the number of protons and the arrangement of the electrons. The unique atomic structure of each element results in unique, elemental specific emission lines.
- 3.24 Spectra or emission spectra are recorded values of the wavelengths and intensity of electromagnetic radiation emitted during electronic transitions.
- 3.25 A Spectrometer is a device for detecting and analyzing the wavelenghts and intensity (spectra) of electromagnetic radiation.
- 3.26 Structure relates to the arrangement of the internal components of an aggregate material and can include the subatomic structure, which in general involves electrons, quantum states, nuclei and their interactions; the atomic structure, which involves the organization of atoms and molecules; the microscopic structure, which includes agglomerations of large molecules and atoms into larger units and macroscopic structure that encompass the visually perceptible structure and overall nature of the material.
- Discussion*—The spectral patterns generated during the LIBS process reflect to varying degrees the subatomic, atomic, microscopic and macroscopic nature of the aggregate. The accuracy of this reflection, as it relates to a specific variable, determines how well multivariate models developed will predict the dependent variable.
- 3.27 SLT operator refers in this practice to the technician or engineer who introduces the target aggregate into the laser scanning system; and operates the system.
- 3.28 Training set is a set of spectra associated with aggregate materials from known sources with known properties that are used to calibrate a chemometric model.
- 3.29 True value refers to a sample variable measured by a known test method that determines the correct value associated with the specific variable.
- Discussion*—While the correct or true value is typically assumed to have a high degree of accuracy, this is not necessarily the case and care must be taken to ensure that test methods used to quantify the true value are reliable.

- 3.30 Validation set is a set of spectra associated with aggregate materials from known sources with known properties that are used to test and determine how well the calibrated chemometric model can predict a designated variable.
- 3.31 Visible light corresponds to a wavelength range in the electromagnetic spectrum of approximately 400 to 700 nanometers.

4. SUMMARY OF PRACTICE

The laser scanning process described in this application introduces a methodology that can provide quality control screening in near-real time during aggregate processing or pavement production. The practice requires no special sample preparation and provides the means to characterize aggregate type, quality, source information and engineering material property data. This process is achievable with the use of bulk aggregate laser scanning equipment that can be deployed in the laboratory or in the field. The scanning system employs a high-powered pulsed laser that excites the atoms that make up the aggregate material resulting in the release of electromagnetic radiation with unique spectral lines and patterns. The laser scanning process is referred to as laser-induced breakdown spectroscopy. The unique spectral patterns generated in this process can be equated to fingerprints that reveal information about the underlying structure of the target aggregate material. These unique spectral patterns can be used to assess similarities and differences between aggregates. The spectral patterns of aggregate materials are highly complex and typically contain approximately 14,000 different wavelengths and intensities. Using multivariate analysis or chemometric modeling, however, it is possible to analyze the wavelength patterns and define and discriminate between spectral patterns. By establishing a database of spectra with known properties, it is possible to compare or discriminate the spectra of unknown aggregate materials with known materials and as a result define aggregate type, quality, source and engineering material properties of the unknown materials-based spectral pattern data.

5. SIGNIFICANCE AND USE

- 5.1 Quality control testing to ensure the suitability of aggregate for highway construction relies almost exclusively on laboratory based test methods and specifications compiled by the American Association of State and Highway Transportation Officials (AASHTO), the American Society of Testing Materials (ASTM), or a local jurisdiction. Almost all existing test methods and their corresponding criteria are empirical in nature and are based on studies undertaken over the years that have defined correlations between the results of laboratory test data and field experience. All of the above referenced test methods require sample collection, sample preparation, and sample testing methods that can take hours, days, weeks, and in some cases months to complete. Individual tests must be conducted for each aggregate quality parameter of interest. Finally, for some test methods, for practical reasons, it may not be possible to collect a sufficient size and/or number of samples in accordance with specified statistical criteria (see ASTM E122).
- 5.2 The laser scanning equipment described in this application can be employed in state or private materials testing laboratories to screen samples to ensure that targeted samples are in compliance with appropriate job specifications. Such a system can be employed as a "Smart Tester" to determine whether or not additional, specification-linked laboratory testing of the aggregate material is required to prioritize laboratory testing resources for more efficient operations. Near-real time feedback to regulators, aggregate producers or asphalt or Portland cement manufacturers introduces a level of quality control not available using current practices.
- 5.3 The scanning process provides the means to determine multiple engineering material properties with one scan, thereby minimizing or eliminating or minimizing the need for multiple tests to characterize the material.
- 5.4 The large sample sizes that can be scanned with the laser equipment in a short time period (i.e., approximately 3 gallons per sample in a 30 minute time period) provide greater assurance that the samples tested are representative of the source material.

- 5.5 The near-real time feature of this application substantially reduces the risk that substandard materials will be incorporated into highway materials reducing the short term costs associated with the removal of below standard pavement structures, when such below standard materials are detected; and the longer term life cycle costs due to the undetected use of substandard materials.

6. MODEL DEVELOPMENT AND PRODUCTION MONITORING PROCEDURES

- 6.1 Prior to the production monitoring stage, where aggregates are monitored on a regular basis, multivariate or chemometric models to be used in the screening process must be calibrated and validated for specific target properties. After this step is achieved then the application can be employed in the production monitoring stage.
- 6.2 The first step in the model development stage requires the collection of a sufficient number of aggregate samples and the development of a sufficient spectral data database (spectral library) to calibrate selected multivariate models. Aggregate samples collected during this process should be collected and reduced to the appropriate sample size for scanning in accordance with AASHTO T2 and AASHTO T248, respectively.
- Note 1** – The final samples size for the laser scanning system described below is 11.4 to 13.9 liters (3 to 4 gallons).
- 6.3 The types and number of aggregate samples collected during the model development stage (calibration set) need to be such that the aggregate sources span the range of values for the specific properties being modeled so that sufficient data are available for the model to accurately resolve spectral pattern difference between samples with different property values
- 6.3.1 As an example, it may be of interest to differentiate between samples that fail a defined test (e.g., D-cracking test) from those that pass the test. This is a form of discriminant analysis. The spectral data from the known samples are used to discriminate between two types of samples (i.e., passing and failing). A sufficient number of samples must be collected that exhibit passing and failing properties.
- 6.3.2 Alternatively, the goal may be to determine the LA loss of an unknown sample. In this case data development would entail the collection of samples that exhibit known LA loss values that encompass the range of loss values of interest. This is sometimes referred to as compositional modeling, since the goal of the model is to predict a specific value or composition; in this case percent loss.
- 6.3.3 The number of samples required to develop an adequate spectral library is critical and will depend on the specific property of interest and the heterogeneity of the aggregate samples being tested. As a rule of thumb, it is recommended that a minimum of 30 samples of each sample type be run before proceeding with the model calibration process. Additional samples may be needed after the initially developed models are evaluated.
- 6.4 During model development, the scanned spectra will be introduced into multivariate models (e.g., principal component analysis or partial least square regression) so that the selected chemometric models can "learn" what the spectrum of a sample looks like. This calibration process is sometimes referred to as "training" the model. The set of samples used in this calibration process is commonly referred to as the "training set."
- Note 2** – A detailed mathematical description of model types is presented in ASTM 1655.
- 6.5 Model validation, which follows model calibration, is the process of testing the calibrated model to determine how well, the model can predict the desired model output. Testing of a calibrated model is typically undertaken with spectral data from a new aggregate sample set that differs from the calibration training set described above. This new sample set is sometimes referred to as a "validation set." The total number of samples collected for use in the validation set is subject to the discretion of the data analyst and the analyst's confidence in the model accuracy.
- 6.6 Production monitoring can proceed after the model's accuracy is judged acceptable.
- Note 3** – A detailed description of multivariate modeling validation procedures is presented in ASTM 2617.

7. SAMPLING LASER AND TARGETING SYSTEM EQUIPMENT

- 7.1 The laser scanning equipment designed for bulk scanning of aggregates described in this practice is referred to as the Sampling Laser and Targeting System (SLT).
- 7.2 The SLT is a bulk laser scanning system. It is designed to provide for continuous or semi-continuous monitoring of a bulk stream of material. The SLT can be used as a stand-alone unit in a materials laboratory, where sample buckets are deposited into the system, or it can be deployed adjacent to a moving conveyor line of bulk material, where a subsample of the target material is diverted into the SLT for analysis.
- 7.3 The System consists of five integrated systems, illustrated in Figure 1. These systems are referred to as the 1) Material Flow System, 2) Laser Targeting System, 3) Laser-Optics System, 4) Data Communication and 5) Control System.

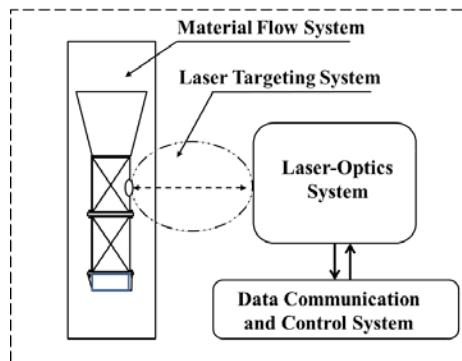


FIGURE 1 General SLT schematic.

- 7.4 The five integrated systems are enclosed in an environmentally controlled steel cabinet on rollers with dimensions of approximately 4 ft. high, 2 ft. wide and 3 ft. long. A photograph depicting an operator pouring an aggregate sample into the top of this enclosed cabinet is shown in Figure 2.
- 7.4.1 The material flow system is comprised of an aggregate feed hopper, a material flow chute and an aggregate collection chamber. The aggregate is fed into the feed hopper and transported vertically downward through the material flow chute and deposited in a receptacle (bucket) in the aggregate collection chamber.
- 7.4.2 The laser optics system contains the laser, the laser power supply and environmental control system and the spectrometer that receives the emission generated by the laser pulse.
- 7.4.3 The laser targeting system directs the laser pulses, by means of a series of lenses and mirrors, through a pressurized dust control system to a small orifice in the materials flow chute. This orifice exposes the aggregate flowing through the material flow chute to the laser beam. The system includes a fiber optic cable that transmits the light from the laser-induced plasma back to the spectrometer, located in the laser-optics system, which receives and resolves the light transmitted by the fiber optic cable into its characteristic spectra.



FIGURE 2 Operator feeding aggregate sample into enclosed SLT cabinet.

- 7.4.4 The computer control system consists of a computer, a programmable logic controller, and a Human to Machine (HMI) interface monitor, to coordinate the aggregate flow, laser, spectrometer and environmental control operations.
- 7.4.5 The data processing system collects the spectral data in the local computer and transmits the data to a remote central data processing station where the chemometric models analyze the data and return the results to the local SLT computer for operator viewing.

Note 4—The referenced laser scanning system is referred as the Sampling Laser and Targeting System (SLT). A more detailed description of this system can be found elsewhere (see NCHRP 168, 2015).

8. SAMPLING LASER AND TARGETING SYSTEM PERSONNEL

- 8.1 SLT operations require the integrated efforts of designated personnel to operate and maintain the system and to provide data analysis. These personnel are referred to as the SLT operator, maintenance engineer and data analyst.
 - 8.1.1 The SLT operator is the local technician or engineer who processes the target aggregate through the laser scanning system; and operates the system. The operator logs into the system computer, inputs into the computer a pre-selected sample identifier code, identifies the type of model to be run, processes the sample, and performs light maintenance activities.
 - 8.1.2 The maintenance engineer refers in this practice to the engineer or technician responsible for maintaining the laser scanning system.
 - 8.1.3 The data analyst is the person(s) responsible for analyzing the data, calibrating and validating the models.
- 8.2 The level of expertise for each designated person is as follows:
 - 8.2.1 SLT operator—in-house material lab technician with some special training in the operation and simple maintenance procedures for the laser scanning system.
 - 8.2.2 Maintenance engineer—more detailed training on the internal components and troubleshooting procedures for the laser scanning system with equipment. Could be trained in-house technician with manufacturer support.
 - 8.3.3 Data analyst—experienced computer and multivariate modeling expert, typically non-in-house personnel.