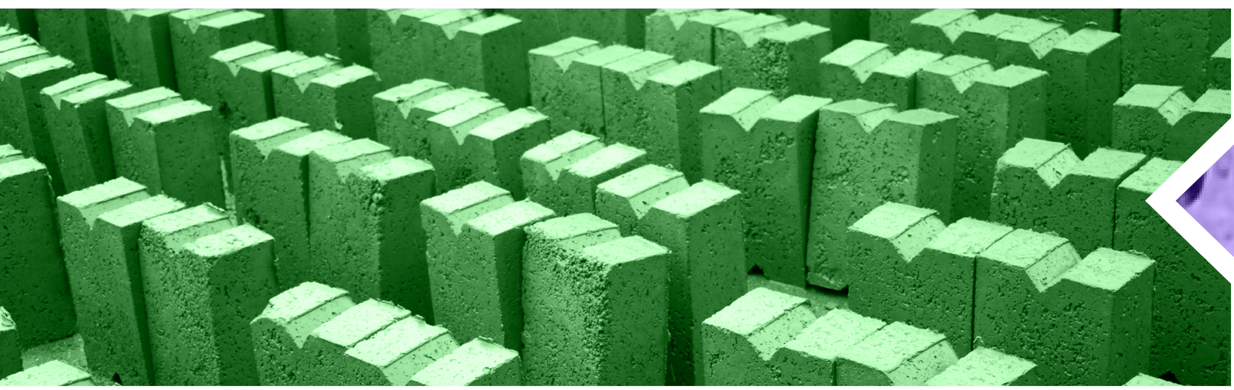
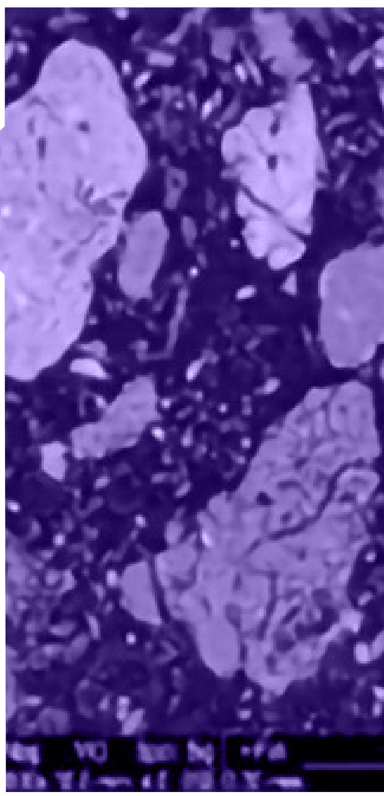
EXPLORATORY ADVANCED RESEARCH

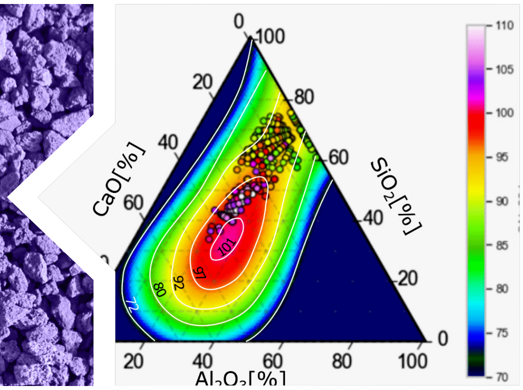
Exploratory Advanced Research Program

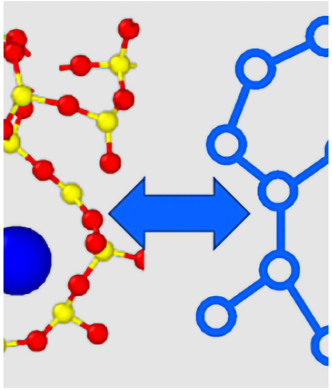
Machine Learning and Pozzolans for Concrete for Highway Pavements and Structures

WORKSHOP SUMMARY REPORT









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16. Abstract

On December 14 and December 15, 2020, the Federal Highway Administration's (FHWA) Office of Infrastructure Research and Development held a virtual workshop called "Machine Learning and Pozzolans for Concrete Infrastructure Materials" with 80 participants in attendance. The workshop, consisting of eight presentations, largely focused on three ongoing Exploratory Advanced Research Program projects and one National Cooperative Highway Research Program project related to the pressing issue of finding new sources of supplementary cementitious material (SCM) for use in concrete for our Nation's roadway infrastructure.

For decades, fly ash, a by-product of coal plants' power-generating process, has been an important source of SCM for highway infrastructure concrete, enhancing the performance, economic feasibility, durability and sustainability of cement mixtures containing ordinary portland cement. As a result of environmental regulations and a general transition of power utilities' fuel source from coal to natural gas in recent years, high-quality fly ash has become increasingly scarce. In response, FHWA organized a workshop to illustrate ongoing research related to the pursuit of fly ash alternatives to ensure the sustainability of our Nation's roadway infrastructure.

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Executive Summary

On December 14 and December 15, 2020, the Federal Highway Administration's (FHWA) Office of Infrastructure Research and Development held a virtual workshop called "Machine Learning and Pozzolans for Concrete Infrastructure Materials" with 80 participants in attendance. The workshop, consisting of eight presentations, largely focused on three ongoing Exploratory Advanced Research (EAR) Program projects and one National Cooperative Highway Research Program (NCHRP) project related to the pressing issue of finding new sources of supplementary cementitious material (SCM) for use in concrete for our Nation's roadway infrastructure.

For decades, fly ash, a by-product of coal plants' power-generating process, has been an important source of SCM for highway infrastructure concrete, enhancing the performance, cost, and sustainability of mixtures containing ordinary portland cement (OPC). As a result of environmental regulations and a general transition of power utilities' fuel source from coal to natural gas in recent years, high-quality fly ash has become increasingly scarce. Many of the presentations from this FHWA workshop illustrated ongoing research related to the pursuit of fly ash alternatives to ensure the sustainability of our Nation's roadway infrastructure.

The first day of the workshop consisted of the following presentations:

- "Physically Informed Data-Driven Methods for Greatly Enhancing the Use of Heterogeneous Supplementary Cementitious Materials in Transportation Infrastructure" given by Dr. Mathieu Bauchy.
- "Performance-Based Classification Methods for Reclaimed Fly Ash in Concrete" given by Dr. Tyler Ley.
- "Using ANN (Artificial Neural Networks) in Analysis and Design of Airfield Concrete Pavements" given by Dr. Adel Rezaei Tarahomi.
- "Use of Artificial Intelligence in Characterizing Paving Materials" given by Dr. Raj Dongre.

The second day of the workshop consisted of the following presentations:

- "Rapid Screening of Reactive Fly Ashes By Machine Learning" given by Dr. Mathieu Bauchy.
- "Performance-Based Classification Methods for Reclaimed Fly Ash in Concrete" given by Dr. Tyler Ley.
- "Nontraditional and Natural Pozzolan-Based SCMs or Inorganic Polymers for Transportation Infrastructure" given by Dr. Jan Olek, Dr. Farshad Rajabipour, and Dr. Sulapha Peethamparan.
- "Recommendations for Revision of AASHTO M 295 Standard Specification to Include Marginal- and Unconventional-Source Coal Fly Ashes" given by Dr. Lisa Burris and Dr. Prannoy Suraneni.

Each presentation included a question-and-answer session, and, throughout the workshop, speakers engaged in FHWA-facilitated general discussion about issues related to fly ash and data analysis techniques brought up during the presentations.

Part 1: Speaker Presentations

Physically Informed Data-Driven Methods for Greatly Enhancing the Use of Heterogeneous Supplementary Cementitious Materials in Transportation Infrastructure

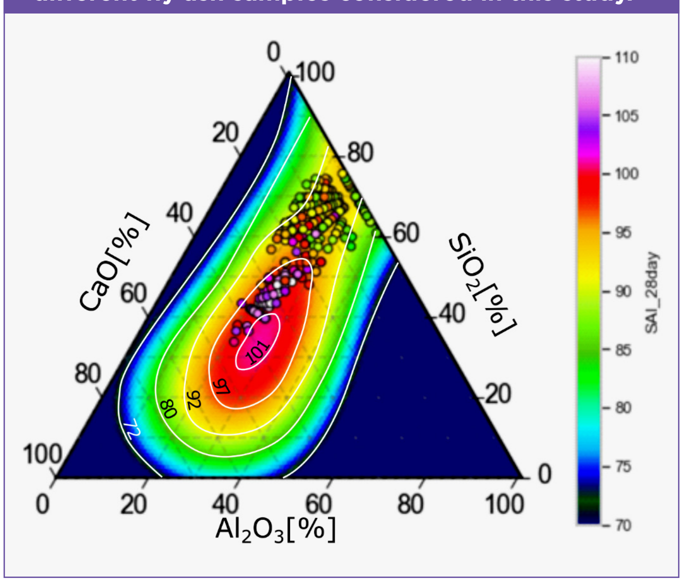
Dr. Bauchy, an associate professor at the University of California-Los Angeles (UCLA) and co-primary investigator of the EAR Program project "Physically Informed Data-Driven Methods for Greatly Enhancing the Use of Heterogeneous Supplementary Cementitious Materials in Transportation Infrastructure," spoke about a machine-learning model for assessing fly ash's strength activity index (SAI) developed in the EAR Program study.

Dr. Bauchy's EAR Program project employs machine learning and the use of artificial intelligence tools and programs to analyze large quantities of data, to understand which sources and characteristics of fly ash can be used successfully in the production of concrete for highway infrastructure projects. Overall, the researchers of this project want to understand the fly ash chemical properties that influence its performance in concrete. Such insights could allow the use of diverse fly ashes in concrete without sacrificing the mixture's engineering performance.

The machine-learning model for assessing fly ash SAI that Dr. Bauchy discussed is a significant step in achieving the aims of the EAR Program project's goals. The ability of fly ash to replace OPC in concrete is typically assessed based on its SAI. However, the physical and chemical characteristics of fly ash that dictate its SAI and, more generally, suitability to replace OPC have remained largely unidentified. This phenomenon limits the use of high-volume fly ash replacement.

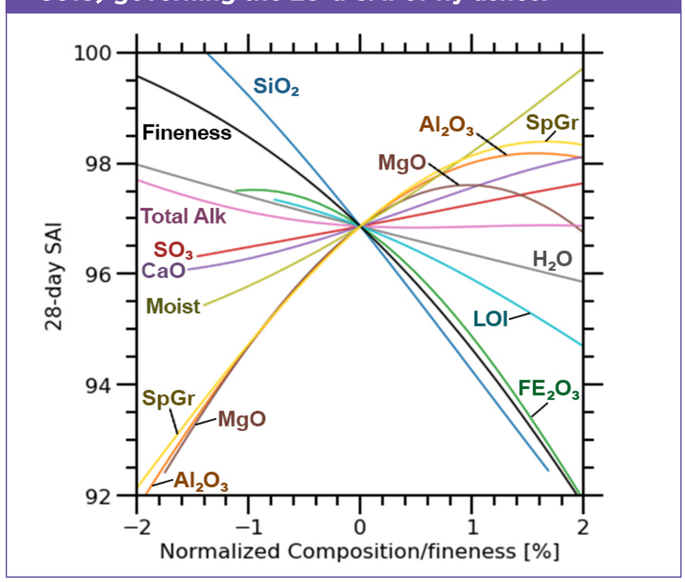
Based on the analysis of a one-of-a-kind large dataset including more than 22,000 fly ash compositions (covering both the Class C and F domains), the EAR Program study researchers have developed a machine-learning model that maps the fineness and chemical composition of fly ash to its SAI. This model successfully predicts the SAI of a wide array of fly ashes with unprecedented accuracy. The model is also able to analyze how fineness and individual oxides contribute to fly ashes' ability to replace cement. Further information about the project's research can be seen in figure 1 and figure 2.

Figure 1. Image. AI-based prediction of the SAI within the calcium-aluminate-silicate space for the different fly ash samples considered in this study.



CaO = calcium oxide; Al_2O_3 = aluminum oxide; SiO_2 = silicon dioxide.

Figure 2. Graph. AI-based interpretation of the influence of the individual features (per ASTM C618) governing the 28-d SAI of fly ashes.



SO_3 = sulfur trioxide; MgO = magnesium oxide; Fe_2O_3 = iron (III) oxide; H_2O = water; SpGr = specific gravity; LOI = loss on ignition.

Performance-Based Classification Methods for Reclaimed Fly Ash in Concrete

Dr. Ley, a professor at Oklahoma State University and primary investigator of the EAR Program project "Performance-Based Classification Methods for Reclaimed Fly Ash in Concrete," discussed the machine-learning aspects of his study.

Much of the fly ash used in concrete production meets current specifications. However, older "reclaimed" fly ash, located in landfills and impoundments, has potential value as well, as an effective SCM. Dr. Ley's project focuses on assessing how reclaimed fly ash may perform when used for concrete production and the differences in chemical composition of various reclaimed fly ashes.

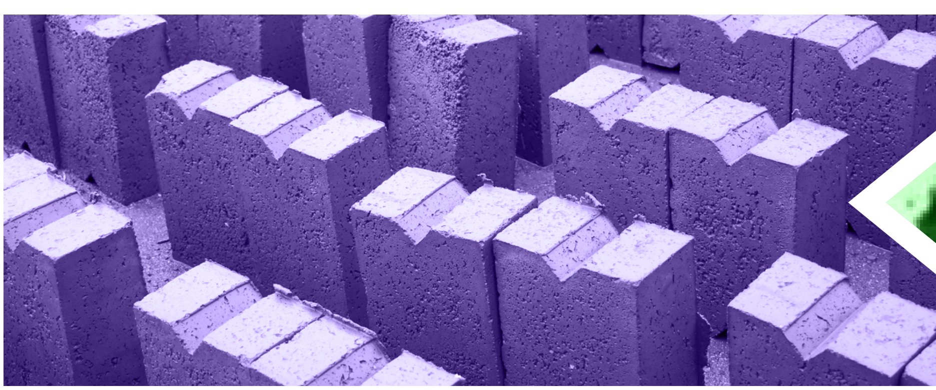
Using Artificial Neural Networks in Analysis and Design of Airfield Concrete Pavements

Dr. Rezaei Tarahomi, an FHWA Turner-Fairbank Highway Research Center research associate, discussed his study on developing an artificial neural network (ANN) tool to replace and reduce the computing time of typical finite-element method (FEM)-based software. This ANN tool is able to predict stresses and deflections of airport concrete pavements at a faster rate than the traditional FEM model. The tool can determine the suitable thickness of an airfield concrete pavement based on given design variables (such as the expected type of aircraft landing on the airfield). The study's data came from finite-element simulation, using 124 computers to conduct 700,000 simulations with 165 types of airplanes.

Use of Artificial Intelligence in Characterizing Paving Materials

Dr. Dongre, a private laboratory researcher and consultant, gave an overview of ANN modeling developed for characterizing asphalt binders used in paving mixtures.

One ANN model developed, trained from a database of more than 800 types of asphalt from the United States and around the world, can predict the performance grade (PG) of asphalt. The model is a machine-learning gradient boost type of model that uses parameters calculated from the creep-recovery test data as input variables to predict both high and low PG. The ANN model's training database is diverse and encompasses all PGs of asphalt binders currently in use in the United States and the rest of the world. The asphalts included in the database were sourced from multiple State departments of transportation in the United States and several suppliers in Europe, Asia, and the Middle



East, as well as the Strategic Highway Research Program materials library. A separate database was created and trained for Utah because Utah follows a slightly modified version of the Association of American State Highway and Transportation Officials (AASHTO) PG system.

Another ANN application predicts hot mix dynamic modulus (E^*) from mix gradation inputs, effective binder content, and air voids. The ANN-based model predicted E^* within 10 percent of the measured value. To predict the complex modulus (G^*) and phase angle of rolling thin-film oven-aged binder requires additional data inputs, the frequency and temperature of interest.

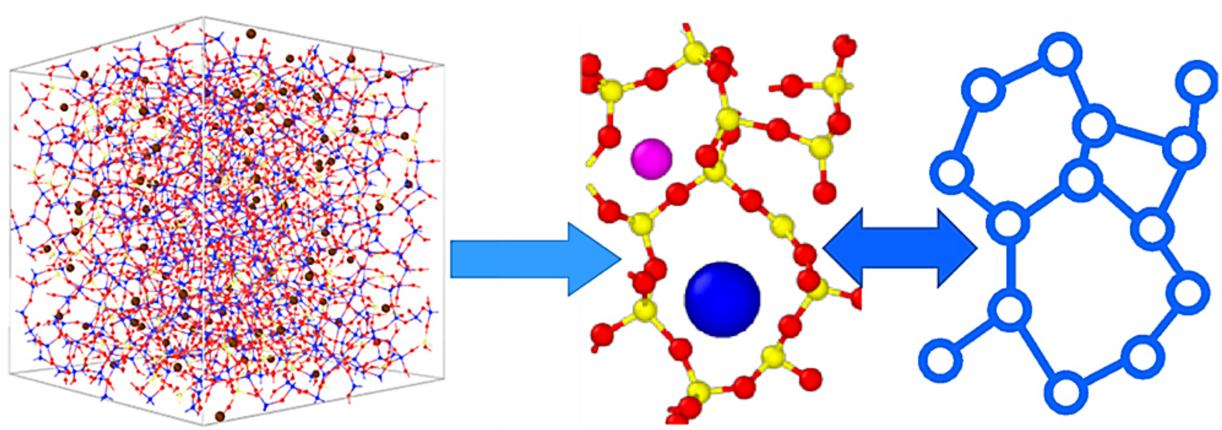
Rapid Screening of Reactivity of Fly Ashes by Machine Learning

Dr. Bauchy gave an additional presentation related to the UCLA EAR Program project about the creation of an ANN model that accurately predicts the weight of fly ashes' amorphous phase and the network topology, an indicator of the reactivity.

The use of fly ash in concrete has thus far been limited to replacement levels of less than 20 percent by weight due to uncertainties in its performance as SCM. The ability of fly ash to replace cement in concrete is largely determined by the reactivity of fly ash's amorphous phase, a time when chemical reactions lead to the strengthening of the material (figure 3). Characterizing the amorphous phase is complex and costly, which limits practical screening of large amounts of fly ashes needed to substantially increase the percentage and types of fly ash suitable as SCMs.

To deal with this issue, the EAR Program study researchers have introduced a machine-learning-based methodology that enables robust screening of reactive fly ashes based solely on fast, inexpensive bulk characterization by using the distribution of fly ashes during the amorphous phase as a structural proxy for their reactivity. Trained from a dataset of more than 100 fly ashes (a large proportion of the available fly ashes in the U.S. market), the ANN tool can maximize the beneficial use of fly ashes obtained from industrial production, as well as identify opportunities for the reclamation of ashes that are presently stored in impoundments.

Figure 3. Image. Atomic-scale structural origin of fly ash strength reactivity.



Note: The amorphous phase in fly ashes presents a disordered atomic structure (similar to aluminosilicate glasses) that controls their reactivity. The reactivity of the amorphous phase in fly ashes is encoded in their atomic topology.

Performance-Based Classification Methods for Reclaimed Fly Ash in Concrete

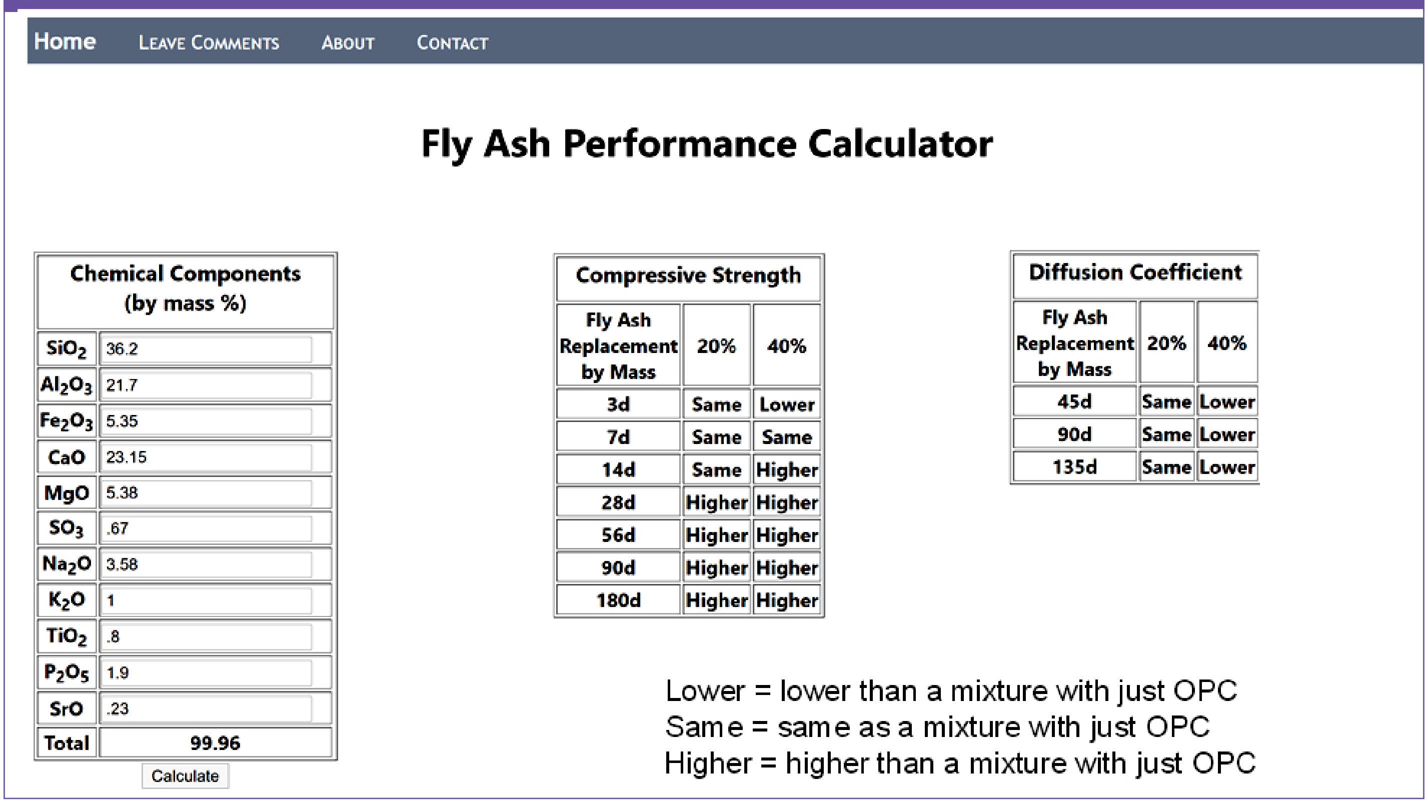
Dr. Ley gave a second presentation related to his EAR Program project. This talk focused on the materials and physical test results to date of his team's study. He also highlighted some of the additional characterization work and durability testing that is planned at the cooperating universities. Dr. Ley has created a preliminary fly ash performance calculator in which researchers can enter data about the bulk chemical components of the materials and using a comparison with other reactivity results suggest potential strength of the concrete.(1) This website uses a machine-learning algorithm to predict the strength and diffusion coefficient. Instead of giving precise predictions, the algorithm predicts if the properties are higher, lower, or the same as a mixture with only portland cement. An image of the fly ash performance calculator can be seen in figure 4.

Nontraditional and Natural Pozzolan-Based SCMs or Inorganic Polymers for Transportation Infrastructure

Dr. Olek, a professor at Purdue University, Dr. Rajabipour, a professor at Penn State, and Dr. Peethamparan, a professor at Clarkson University, spoke about their work related to the EAR Program project "Nontraditional and Natural Pozzolan-Based SCMs or Inorganic Polymers for Transportation Infrastructure." Their study seeks to understand how nontraditional and natural pozzolan (NNP) might perform in concrete transportation infrastructure, facilitating the process of using NNP as an SCM on an industrial scale in the future.

NNPs such as volcanic ashes, lower-purity calcined clays, ground bottom ashes, and fluidized bed combustion ashes, which are nontraditional pozzolans, provide a similar pozzolanic reaction and can be used to improve concrete properties, serving as a possible

Figure 4. Image. Fly ash performance calculator.(2)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Fly Ash Performance Calculator

Chemical Components (by mass %)	
SiO_2	36.2
Al_2O_3	21.7
Fe_2O_3	5.35
CaO	23.15
MgO	5.38
SO_3	.67
Na_2O	3.58
K_2O	1
TiO_2	.8
P_2O_5	1.9
SrO	.23
Total	99.96

Calculate

Compressive Strength		
Fly Ash Replacement by Mass	20%	40%
3d	Same	Lower
7d	Same	Same
14d	Same	Higher
28d	Higher	Higher
56d	Higher	Higher
90d	Higher	Higher
180d	Higher	Higher

Diffusion Coefficient		
Fly Ash Replacement by Mass	20%	40%
45d	Same	Lower
90d	Same	Lower
135d	Same	Lower

Lower = lower than a mixture with just OPC
Same = same as a mixture with just OPC
Higher = higher than a mixture with just OPC

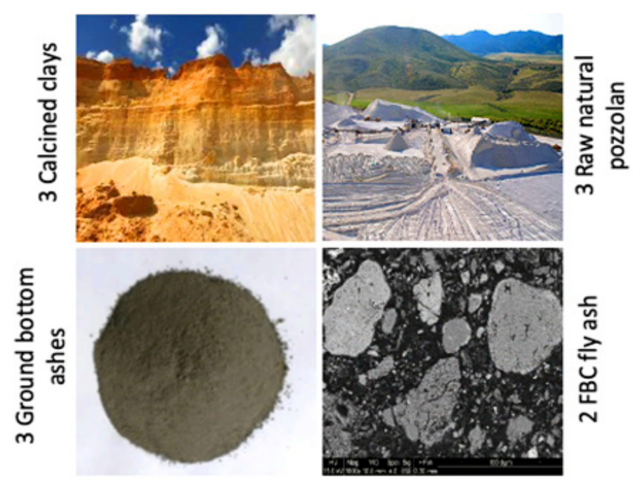
SCM alternative to fly ash. They are produced in abundance throughout the United States and are cost competitive.

The first phase of the study identified viable sources from across the United States, characterized the chemical and physical properties of these SCMs, and determined how these properties might be optimized for performance in concrete. Aspects of their research work can be seen in figure 5, figure 6, and figure 7. Table 1 illustrates the data given in figure 7.

Recommendations for Revision of AASHTO M 295 Standard Specification to Include Marginal- and Unconventional-Source Coal Fly Ashes

Dr. Burris, a professor at Ohio State University, and Dr. Suraneni, a professor at the University of Miami, spoke about their work in the NCHRP project "Recommendations for Revision of AASHTO M 295 Standard Specification to Include Marginal- and Unconventional-Source Coal Fly Ashes." This project aims to evaluate marginal- and unconventional-source fly ash and provide updated recommendations for their inclusion in the AASHTO M 295 standard specification.(2)

Figure 6. Image. Four classes of NNPs studied in this project.



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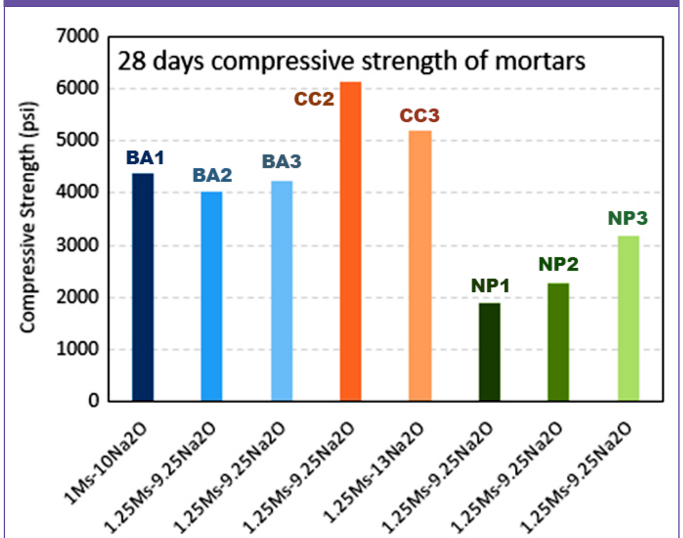
FBC = fluidized bed combustion.

Figure 5. Graph. A comparison of compressive strength of mortars prepared from alkali-activated NNPs using optimized compositions of alkaline solutions.



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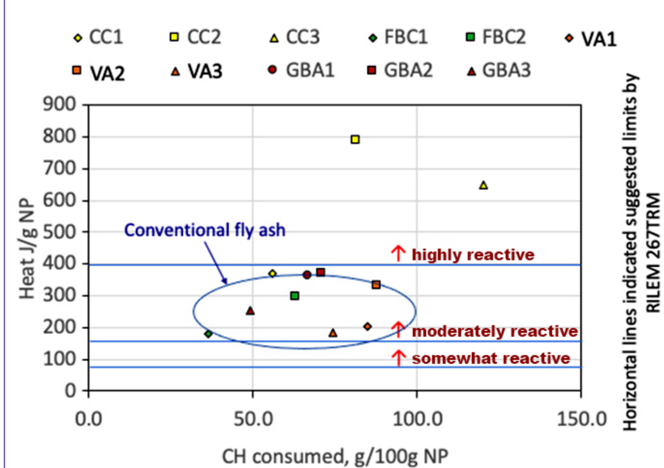
BA = bottom ash; CC = calcined clays; Ms = silicate modulus; Na2O = sodium oxide; NP = natural pozzolan.

Figure 7. Graph. Reactivity of the 11 NNPs as measured by ASTM C1897 (R3 test).



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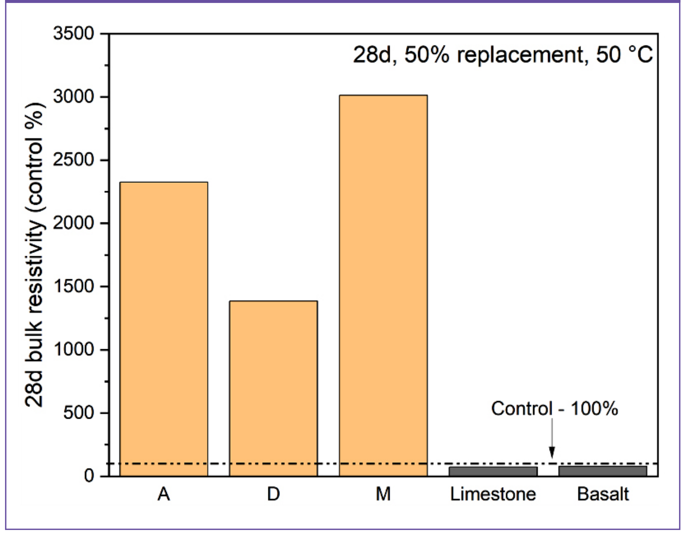
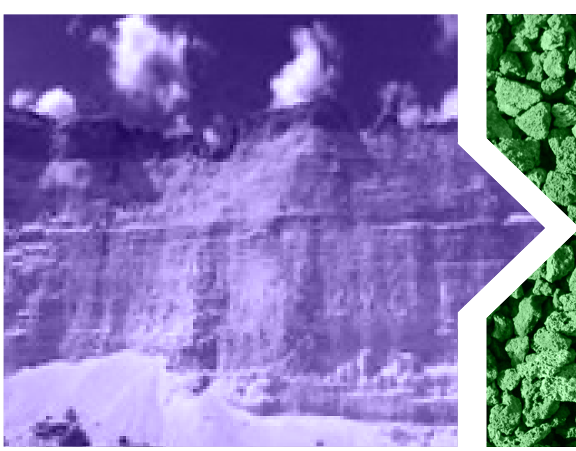
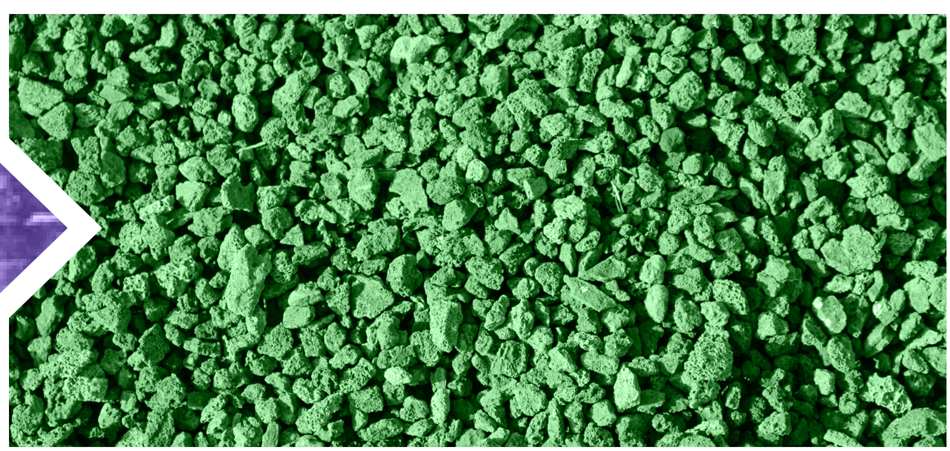
CC = calcined clay; CH = calcium hydroxide; FBC = fluidized bed combustion; GBA = ground bottom ash; RILEM = International Union of Laboratories and Experts in Construction Materials, Systems and Structures; TRM = Test for Reactivity of Materials; VA = volcanic ash.

The speakers presented preliminary results for unconventional fly ashes, including characterization, reactivity, adsorption, and effects on cement pastes, mortars, and concrete. Issues with current specifications, including the SAI test, were clearly highlighted. The development of new test methods could result in updated AASHTO specifications, allowing for the use of a broader range of quality materials such as unconventional-source fly ash. A graph related to the study can be seen in figure 8.

Figure 8. Graph. Bulk resistivity measurements at 50 °C and 50 percent SCM replacement are clearly able to distinguish between reactive fly ashes (A, D, M) and inert fillers (limestone, basalt).







Part 2: Conclusions

The workshop included general discussions in which speakers answered questions about the various research projects presented. From these discussions, workshop participants drew several conclusions, including the benefit of performance-based specifications for SCMs as opposed to specifying the chemical composition of materials used for concrete cement. This change would mean revising the AASHTO specifications regarding the use of fly ash and other SCMs in concrete. Performance-based specifications would include expectations about how SCMs perform against alkali silica reactivity (which is an interaction between the cement and aggregates that can cause the concrete to swell, crack, and break apart), the amount of water needed for the mix, and the ability to maintain entrained air, which improves the durability of concrete cement, especially in areas with freezing temperatures.

Discussions noted that the definition of reactivity is inconsistent in the research projects presented. Some projects look at the reactivity of SCMs at very early ages (less than 7 days), while others look at reactivity at later ages. This difference has also led to differences in reactivity tests, namely tests that are conducted at different pH levels. The pH level influences reactivity. So if reactivity is going to be a performance metric, the concrete materials research community needs to come to a consensus on how it should be tested and reported.

Discussions also touched on the concerns of concrete producers. For use in concrete, producers need to have confidence that the SCM is consistent. Consistency is currently measured by loss on ignition (a process that helps determine water content and/or carbonation that could harm the mixture's quality), moisture content, and particle size on a 300-µm sieve. These may or may not be the best parameters, but concrete producers seem to be comfortable with them at this point.

The discussions brought up the idea of regional concrete mixtures in the United States that utilize the most prevalent types of SCM produced nearby. Such a model could serve as a reference mixture for particular fly ash and might be a good tool to evaluate a potential SCM. This approach to evaluating SCMs would give a quick indicator as to how the mixture with the candidate material might have to be engineered to achieve the desired properties.

Finally, discussion participants found that additional efforts to educate and reach out to concrete producers and end users about these efforts are needed. Concrete specifiers, factory owners, and end users should consider the following questions to identify the needs and approaches to expand sustainable and high-performing SCM options to use in highway infrastructure projects:

- Is there interest in a performance-based approach for each type of SCM (where each type of SCM has a certain performance specification)?
- Is there interest in an approach that provides an indicator of the mechanical properties of different SCMs?
- Is there interest in an approach that provides an indicator for the durability performance of a new SCM?
- Is there more interest in a modeling or an empirical approach that could give a quick indicator of SCM viability, or would a complete panel of physical test data for every new SCM be preferable?

Appendix A

Table 1. Reactivity of the 11 NNPs as measured by ASTM C1897 (R3 test).

Material	Heat J/g NP	CH Consumed g/100g NP
CC1	372	56
CC2	793	81
CC3	646	120
FBC1	181	37
FBC2	301	63
VA1	205	85
VA2	338	88
VA3	182	75
GBA1	368	66
GBA2	376	71
GBA3	250	49

CC = calcined clay; CH = calcium hydroxide; FBC = fluidized bed combustion; GBA = ground bottom ash; NP = natural pozzolan; VA = volcanic ash.
Note: somewhat reactive threshold = 75 J/g NP; moderately reactive threshold = 160 J/g NP; highly reactivity threshold = 400 J/g NP.

References

1. Tyler Ley. n.d. “Fly Ash Performance Calculator” (web page). http://flyash.herokuapp.com/.

2. American Association of State Highway and Transportation Officials. 2019. *Standard Specification for Coal Fly Ash and Raw or Calcined Natural Pozzolan for Use in Concrete*. AASHTO M 295. Washington, DC: American Association of State Highway and Transportation Officials.

Getting Involved with the EAR Program

To take advantage of a broad variety of scientific and engineering discoveries, the EAR Program involves both traditional stakeholders (State department of transportation researchers, University Transportation Center researchers, and Transportation Research Board committee and panel members) and nontraditional stakeholders (investigators from private industry, related disciplines in academia, and research programs in other countries) throughout the research process.

Learn More

For more information, see the EAR Program website at https://highways.dot.gov/research/exploratory-advanced-research. The site features information on research solicitations, updates on ongoing research, links to published materials, summaries of past EAR Program events, and details on upcoming events.

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