Roadmap for the Development of Advanced Atomization and Spraying Technologies

March 2017
ABOUT THIS ROADMAP

Advanced atomization and spray technologies play a significant role in a wide range of U.S. materials manufacturing and value-added end user industries—approximately 21,500 U.S. companies currently rely on these technologies in their operations while producing $1.91 trillion in goods and employing more than 2.5 million people (U.S. Census Bureau 2014). Advances in atomization and spray technologies have the potential to improve the efficiency, productivity, and global competitiveness of these industries. However, significant technical challenges inhibit faster development and deployment of these innovative technologies.

ASM International recognized the opportunity for a comprehensive roadmap to guide coordinated technology development and implementation efforts to advance atomization and spray technologies. Funded by the National Institute of Standards and Technology (NIST) Advanced Manufacturing Technology Consortia (AMTech) program, now part of NIST’s Manufacturing USA program, this roadmap draws on the expertise of key stakeholders and subject matter experts from across the atomization value chain. The roadmap identifies key activities that will expand the range of advanced atomization and spray technologies available to meet the growing needs of manufacturing industries during the next 10 years.

This roadmap was developed under the direction of Scott Henry, Senior Content Engineer at ASM International, and the technical leadership team of the Atomization Technology Innovation Consortium: James Adams, Iver Anderson, Rob Gorham, Vincent McDonell, Robert Miller, Scott Parrish, Paul Sojka, and Todd Palmer. Subject matter experts and other stakeholders who made essential contributions through phone interviews, workshop participation, and roadmap reviews are also identified in Appendix B of this report. Nexight Group supported the roadmapping process and prepared this roadmap; Greg Hildeman, Ross Brindle, Lindsay Pack, Jared Kosters, and Changwon Suh are the primary contributors.
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Roadmap for the Development of Advanced Atomization and Spraying Technologies
EXECUTIVE SUMMARY

Atomization and spray technologies, which allow for the controlled fragmentation of liquid streams into particles, are integral to a wide range of U.S. industries. Among their many uses, these technologies produce powders for food products, detergents, and pharmaceuticals; provide tailored droplet spray distributions for painting, coating, and spreading agricultural chemicals; enable fuel injection in various combustion processes for heating, jet engines, land-based turbines, and internal combustion engines; and create a variety of metal, ceramic, polymer, and glass powders for use in manufacturing. Approximately 21,500 U.S. companies—93 percent of which are small and medium enterprises—currently manufacture or use atomized powders or rely on the application of specialized sprays that result in the generation of $1.91 trillion in goods and the employment of more than 2.5 million people (U.S. Census Bureau 2014).

Advances in atomization and spray technologies have the potential to further improve the efficiency, productivity, and global competitiveness of many U.S. materials manufacturing and value-added end user industries. For example, technologies that allow for better control of metal atomized powder quality could enable additive manufacturing to become a viable manufacturing technology for increasingly demanding applications in automotive, aerospace, and defense. An increased understanding of viscosity and surface tension could reduce variation in sprayed droplet size and distribution to minimize the amounts of insecticides, herbicides, and fertilizers applied to crops. High-fidelity numerical simulations of fuel injectors could enhance the understanding of how atomized droplets of fuels mix and burn to help improve the efficiency of jet engines.

Figure 1. Impact of Atomization and Spraying Technology
Despite this potential, significant technical challenges currently limit the development and deployment of atomization and spraying technologies in manufacturing applications. These challenges persist due in part to the limited, fragmented approach to funding and conducting atomization and spraying R&D. A more coordinated approach that leverages expertise across industries to address common needs can attract greater resources to advance atomization and spray technologies for everyone who relies on them.

Roadmap Strategy
This roadmap identifies common atomization technology needs across industrial applications, with an emphasis on advanced manufacturing. These needs form an impactful research and development agenda that the Atomization Technology Innovation Consortium is poised to address through collaborative, pre-competitive R&D focused on adding foundational knowledge to underpin and broaden the reach of

Figure 2. Atomization & Spraying Technology Development Pathways
proprietary R&D that individual companies will continue to pursue.

This roadmap organizes collaborative R&D activities into seven technology development pathways. These pathways are driven by end-user needs and combine computational and experimental work to achieve improved control of atomization and spraying processes, resulting in superior powder characteristics and spray performance. Figure 2 illustrates the relationships among the pathways, which aim to achieve the goals that follow.

**P1. Physical Property Data and Standards**

Improve the quality and availability of physical property data and metadata and establish standard measurement and data gathering methods to improve modeling accuracy.

**P2. Process Models**

Develop advanced process models, including models that use high-performance computing systems, to generate more accurate predictions of droplet size and spray patterns based on process parameters.

**P3. Modeling and Numerical Simulations**

Advance the understanding of mechanisms that influence the break-up of fluids by using high performance computing resources, numerical simulation and high-fidelity, physics-based models to refine predictions of the effects of physical property variations, differences in nozzle geometries, and changes in process variables on the characteristics of atomized droplets and spray patterns.

**P4. Diagnostic Methods**

Use advanced diagnostic equipment and techniques—such as laser-based phase Doppler particle analyzers and imaging methods using high-speed cameras, x-rays or high resolution sensors with advanced light technology—to directly observe and measure droplet characteristics (e.g., size, shape, distribution, velocity) and improve atomization processes.

**P5. Real-time Sensors**

Apply existing measurement techniques or develop advanced sensing methods that can be used by researchers to interrogate experimental spray configurations to gather detailed droplet physics information and by industry as robust sensors to obtain real-time data that can be used to adjust atomization and spraying parameters.

**P6. Experimental Test Facilities**

Develop flexible, atomization-focused experimental testing systems that are made available to industry members to conduct collaborative experimental trials that accelerate advancement of atomization and spraying technologies.

**P7. Process Control**

Demonstrate the ability to produce desired droplet or powder characteristics via improved control of atomization or spraying processes during sustained, steady-state, full-scale operating conditions.

**Priority R&D Activities**

This roadmap recommends high-priority research and development (R&D) activities that hold promise for improving atomized powder characteristics and spray performance. While many R&D activities have relevance to both liquid spraying for combustion or coatings and to high-temperature atomization of molten metals for powder applications, the R&D needs shown below are identified by the application (liquid spray or molten metal melt atomization) for which they have primary relevance.
## P1. Physical Property Data and Standards

- Develop a database of Newtonian/non-Newtonian fluid rheological properties, including nozzle and spray characteristics
- Develop a database on thermophysical properties of alloy melts (e.g., surface tension, viscosity, and oxidation rate for process modeling)
- Develop a database of atomization parameters and powder characteristics to facilitate benchmarking and user-friendly alloy modeling
- Perform round-robin testing of powder size across equipment types and measurement procedures

## P2. Process Models

- Develop standardized test case(s) for modeling
- Develop advanced theoretical models to understand the physics of atomization
- Develop physics-based models that can predict the impacts of multi-phase flows with phase changes
- Develop an adaptable, open-source model for molten metal atomization processes

## P3. Modeling and Numerical Simulations

- Conduct engineering-level modeling of the internal injector and spray patterns
- Use direct numerical simulation (DNS) on test case injectors to improve understanding of near nozzle/primary atomization of fluids and aid development of new diagnostic techniques
- Conduct large eddy simulation (LES) of primary atomization with DNS and low-fidelity approaches
- Conduct computational fluid dynamics (CFD) modeling of two-fluid atomization to understand the effect of process parameters on fluid flow and droplet characteristics

## P4. Diagnostic Methods

- Conduct experimental evaluations of spray patterns from standardized test case nozzles with advanced diagnostic equipment
- Characterize dense spray patterns by combining measurement techniques (e.g., digital in-line holography, phase Doppler anemometry [PDA], ballistic imaging, and other interferometric techniques)

## P5. Real-Time Sensors

- Improve existing or develop new diagnostic equipment that are needed for characterization, monitoring, and control of spray processes
- Perform a broad-based gap analysis study to determine sensor needs by industry versus available sensor technologies for process control
- Develop and test robust in-situ sensors and production process control actuators

## P6. Test Facility: Experimental Trials

- Conduct experimental simulations using transparent nozzles to study effects of nozzle geometry, cone angle, internal and ambient pressure, and rheology of fluids on droplet size and dispersion
### Path Forward

Because atomization and spraying technologies are used in a wide range of manufacturing applications, even modest improvements in powder characteristics and spray performance can provide substantial benefits. Widespread increases in efficiency and productivity can help to support a growing and more competitive U.S. manufacturing sector. The R&D activities identified in this roadmap chart the course for future technology advances that, if realized, can accelerate this potential outcome.

To ensure that the coordinated efforts to develop and implement advanced atomization and spray technologies continue to build momentum, ASM International is working with leaders in atomization and spraying to establish the Atomization Technology Innovation Consortium (ATIC). ATIC will serve as an organizing body for cross-industry atomization and spraying technology communities and provide a space for industry and academia to share knowledge and work together to mobilize solutions. By connecting the right people and cultivating a collaborative environment, ATIC will help tap into the nation’s leading expertise to increase control of atomization and spray processes and revolutionize the ways they can be used to drive growth in U.S. manufacturing.
Although scientists and engineers have developed specialized nozzles and unique atomization and spraying methods for a wide range of specific applications, atomization and spray processes can generally be divided into the following two categories:

- **Two-Fluid Atomization and Spray Processes**, including air, inert gas, water, and oil atomization of liquids and melts to form droplet sprays
- **Single-Fluid (Pressure) Atomization and Physically Induced Spray Processes**, including pressurized hydraulic fluid sprays and injectors; centrifugal, vacuum or soluble gas, and ultrasonic atomization; and specialized particulate phase spraying processes, such as thermal spray and spray drying

Figure 4 compares the liquid phase break-up mechanisms of two-fluid and single-fluid atomization and spray processes. Differences among the break-up mechanisms associated with each atomization or spraying process enable the molten or liquid droplet characteristics to be tailored for specific spray applications or to achieve desired atomized powder characteristics. Figure 5 provides an overview of the wide range of applications in which atomization and spray technologies play a significant role.

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**Figure 4. Comparison of Two-Fluid and Single-Fluid Atomization Processes**

<table>
<thead>
<tr>
<th>TYPES OF ATOMIZERS</th>
<th>BREAK-UP MECHANISMS</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Two-Fluid Atomization Processes</strong></td>
<td>Interaction or coupling of energetic fluid to bulk liquid stream or thin film (high superheat) to promote liquid instabilities that evolve into droplets.</td>
</tr>
<tr>
<td>Gas</td>
<td>Molten metal, aqueous solutions, polymers, or glass</td>
</tr>
<tr>
<td>• Inert gas</td>
<td></td>
</tr>
<tr>
<td>• Air (ambient)</td>
<td></td>
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<tr>
<td>• Selected reactive gas</td>
<td></td>
</tr>
<tr>
<td>Water plus evaporation to steam</td>
<td>Molten metal</td>
</tr>
<tr>
<td>Oil plus evaporation to hydrocarbon vapor</td>
<td>Molten metal</td>
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</tbody>
</table>
### TYPES OF ATOMIZERS

<table>
<thead>
<tr>
<th>Two-Fluid Atomization Processes (cont.)</th>
<th>Break-up Mechanisms</th>
</tr>
</thead>
<tbody>
<tr>
<td>Spray drying with pressurized air blast</td>
<td>Agglomerated granules are produced by application of a pressurized air blast to fragment the slurry stream as it is injected into a drying chamber to evaporate moisture.</td>
</tr>
<tr>
<td>Liquid slurry with solid particles and binders</td>
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</tbody>
</table>

### TYPES OF ATOMIZERS

#### Single-Fluid Atomization Processes

<table>
<thead>
<tr>
<th>Pressurized nozzles</th>
<th>Break-up Mechanisms</th>
</tr>
</thead>
<tbody>
<tr>
<td>• Fuel spray nozzles</td>
<td>Sudden release of a pressurized fluid that is discharged into a spray chamber or open environment through orifice, which causes fragmentation of the stream into droplets.</td>
</tr>
<tr>
<td>• Pressurized fluid spray nozzles</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>Spray drying nozzles</th>
<th>Break-up Mechanisms</th>
</tr>
</thead>
<tbody>
<tr>
<td>• Centrifugal (rotating disk)</td>
<td>Agglomerated granules are produced by introducing a slurry onto a rotating disk or by injecting the slurry at high pressure through a nozzle into a drying chamber to evaporate moisture.</td>
</tr>
<tr>
<td>• Pressurized slurry nozzle</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>Centrifugal atomization</th>
<th>Break-up Mechanisms</th>
</tr>
</thead>
<tbody>
<tr>
<td>• Rotating electrode (horizontal axis) with (plasma, e-beam, laser) heated tip</td>
<td>Fragmentation of molten metal is caused by exceeding the balance of the melt surface tension and centrifugal force acting at the periphery of a rotating electrode or disk, which accelerates the molten metal to promote instabilities that evolve into droplets.</td>
</tr>
<tr>
<td>• Rotating disk (vertical axis) with heated or chilled horizontal disk surface</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>Ultrasonic atomization</th>
<th>Break-up Mechanisms</th>
</tr>
</thead>
<tbody>
<tr>
<td>• Whistle-type gas pulse atomization nozzle (Kolsva and Brown-Boveri patents) that promotes periodic melt disintegration</td>
<td>Ultrasonic gas pressure waves or a vibrating surface acting on liquids or molten metals induces high frequency periodic instabilities that evolve into uniform droplets with a narrow size distribution.</td>
</tr>
<tr>
<td>• Drip atomization on vibrating surface to generate aqueous mist of uniform size droplets</td>
<td></td>
</tr>
<tr>
<td>• Vibrating immersed plunger in close proximity to orifice plate to force melt flow through array of holes that creates uniform spherical droplets</td>
<td></td>
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</table>

<table>
<thead>
<tr>
<th>Vacuum or soluble gas atomization</th>
<th>Break-up Mechanisms</th>
</tr>
</thead>
<tbody>
<tr>
<td>• Vertical or upward flow of liquid through a nozzle located between a melting vessel and the spray chamber</td>
<td>Violent expulsion of supersaturated gas from a molten metal stream produces atomized droplets that are discharged into a low pressure spray chamber.</td>
</tr>
</tbody>
</table>

 Courtesy of I. Anderson, Ames Laboratory, August 2015
Figure 5. Applications for Atomization and Spray Technologies

Agriculture

Hydraulic and air-blast nozzles are used to spray chemicals such as insecticides and herbicides on crops, orchards, and forests by aircraft or ground vehicles. Sprays are also used for irrigation to improve crop yield and wash fruits and vegetables before packaging.

Commercial

Pressurized hydraulic nozzles are used to spray water and detergent for car and pressure washing. Sprays are also used in fire suppression—one method generates large water droplets by spraying water at low pressures from fixed sprinkler heads while the other creates atomized water mist droplets by using high pressure water and compressed gas. In addition, several specialized single-fluid spray techniques are used in ink jet printing.

Electric Power and Heat Generation

Coal-fired power plants use scrubbers with limestone slurry sprays to control acid gas and particulate emissions, and use water sprays in their cooling towers. Nozzles are used to inject diesel fuel into the combustion chamber of land-based generators, while atomized water droplets are used to control emissions of NOx. Nozzles are also used to inject atomized fuel oil sprays into combustion chambers in steam boilers.

Healthcare/Medical

Nebulizers are specialized two-fluid atomized spray devices that use a propellant gas or pressurized air to create an aerosol that can be inhaled by people to effectively deliver drugs to a patient's lungs. Cryogenic sprays are also used to produce fine droplets that cool human skin during laser treatments of birthmarks, hair removal, and other skin treatments.

Industrial

Chemical production: Spraying reagents enhance dispersion and to increase liquid-gas mass transfer. Sprays are also used to dry chemicals and washing and rinse solids in filters and centrifuges

Cleaning: Low- and high-pressure nozzles are used to rinse and the inside of clean storage tanks, process equipment, and other surfaces

Manufacturing: Sprays are used for tasks such as applying adhesives, lubricating bearings, and cooling tools during machining operations. Manufactured components and equipment are cleaned and degreased with sprays of hot water and detergent sprays, while in metal manufacturing industries, sprays are applied during rolling for cooling and lubrication.

Metal Production: High-pressure water sprays are used to remove iron oxide scale from steel during rolling, cool metal during casting quench coke from coke-ovens, and rinse pickling solutions.

Metallurgical: Atomized molten metals produce fine grain alloy billets by spray forming. In addition, the nucleated casting process uses low-pressure gas jets to atomize a stream of molten metal droplets enabling large superalloy ingots to be produced with fine grain sizes, minimal segregation, and without oxides.
### Industrial (cont.)

**Mining**: Water sprays are used to reduce coal dust during mining and control dust produced during crushing or grinding of ores, while spray nozzles are used for washing gravel in screening plants.

**Paper manufacturing**: High-pressure sprays are used to debark logs, coat paper, clean rolls, and trim paper.

**Paints and coatings**: Sprays are used to apply paints on automobiles, office furniture, and household appliances, and to apply coatings on glass.

**Waste treatment**: Sprays help aerate wastewater sludge and inject of sludge into high-temperature incinerators.

### Powder Metallurgy and Thermal Spray

**Powder Metallurgy**: Atomization is used to produce metal powders for parts made by pressing and sintering, metal injection molding, and additive manufacturing. Atomized powders are used for coating applications using thermal spray or cold spray techniques, as well as for specialty applications including brake linings, explosives, rocket fuels, solders, conductive paints, and plastics.

**Thermal and Cold Spray**: Spray-dried powders, such as cemented carbides and zirconia-base ceramics used in many high-wear environments, are common feed materials for thermal spray. Ceramic coatings are prominently used as thermal barrier materials on aerospace and land-based gas turbine components.

### Transportation

Sprays generate atomized fuel droplets for jet engine turbines, internal combustion engines, and rocket engines. Highly engineered nozzles are used in internal combustion engines and jet turbines for injecting finely atomized droplets of fuel to enhance evaporation rate to maximize the efficiency and minimize emissions of pollutants (soot, NOx, CO).
STRATEGY FOR ADVANCING ATOMIZATION AND SPRAY TECHNOLOGIES

The strategy presented in this roadmap organizes activities along seven pathways that address the major barriers to advancing atomization and spray technologies across the wide range of industries and applications that use them. Driven by end-user needs, this strategy recognizes the need to focus on a combination of computational and experimental efforts to ultimately achieve the improved control of atomization or spraying processes that will result in superior powder characteristics and spray performance. Figure 6 illustrates the relationships between the seven strategic pathways that are described in more detail below and serves as a framework for organization of the R&D activities that are described under each heading in the roadmap.

Figure 6. Atomization and Spraying Technologies Development Pathways
Roadmap for the Development of Advanced Atomization and Spraying Technologies

P1. Physical Property Data and Standards

Physical properties, such as viscosity and surface tension, are important variables used in physics-based models that simulate the break-up of fluids into droplets and the effect of process parameters on resulting spray and atomization. However, pedigreed physical property data and metadata sets are not widely available, and current methods for measuring and compiling these data can vary across applications. Improving the quality and availability of physical property data and metadata and establishing standard measurement and data gathering methods are necessary to improve modeling accuracy.

P2. Process Models

Process models help researchers better understand and test the different processes that break up fluids and molten metals during atomization and spraying. Although experimental methods such as high speed imaging and x-ray techniques have provided more insight into the nature of dense sprays, advanced models are needed to resolve the fine details of fluid behavior. Developing advanced physics-based process models will result in more accurate predictions of and control over droplet size and spray patterns. In addition, establishing robust atomization models for production that are used by process engineers will improve control of atomization, and enhance the ability to consistently meet powder quality specifications.

P3. Modeling and Numerical Simulations

Numerical simulation and high-fidelity, physics-based models provide far greater detail on the mechanisms that influence the break-up of fluids than traditional process models. Improvements in computational capabilities and broad access to high-performance computing facilities can enable direct numerical simulations of complex engineering spray and atomization processes. Being able to better predict the impacts of variables such as physical property variations, differences in nozzle geometries, and changes in process variables on the characteristics of atomized droplets and spray patterns can enable more advanced process improvements.

P4. Diagnostic Methods

Using advanced diagnostic equipment, such as Doppler particle analyzers and imaging techniques such as high-speed cameras, x-ray or schlieren diffraction imaging enables researchers to directly observe and measure droplet characteristics (e.g., size, shape, distribution, velocity) in response to atomization and spray process variations. Currently, the high cost of diagnostic and imaging equipment and specialized training required to operate the measurement equipment inhibits many companies from using these valuable methods to better understand fluid behavior during atomization. Addressing the challenges of high cost and specialized training will facilitate the use of diagnostic and imaging techniques. Lower cost, easy-to-use equipment will enable researchers to increase the use of diagnostic and imaging equipment apply to their experimental work that will ultimately improve atomization and spray processes.

P5. Real-time Sensors

The availability of advanced sensing and measurement techniques has made real-time data collection and process adjustment a reality
for a wide range of technologies and industries. Applying existing measurement techniques or developing advanced sensing methods could enable faster, more accurate adjustments to atomization and spraying parameters. Sensors can be used by researchers to interrogate experimental spray configurations and to gather detailed droplet physics information for ranking of the most critical control parameters, enabling precise control and improved output of processes.

**P6. Experimental Test Facilities**

Conducting experimental trials at test facilities equipped with advanced diagnostic equipment and staffed with experts is ideal not only for demonstrating the effectiveness of technologies and techniques, but also for sharing results with researchers working in the field. Currently, there are few experimental test facilities dedicated to atomization, and the experimental testing that does take place occurs at different existing facilities, making it difficult to cross-compare results and benefit collectively from the knowledge gained. Developing experimental testing techniques and training for industry members and establishing this capability at new atomization-focused test facilities will be critical for conducting collaborative experimental trials that could help accelerate the advancement of atomization and spraying.

**Areas of Common Ground between Atomization and Spraying**

While this roadmap identifies numerous activities that apply to spraying of liquids or atomization of molten metals, it is important to note that these technologies share many areas of common ground that provide the basis for crosscutting collaborative R&D in science and technology. The following examples are intended to highlight research activities that address fundamental understanding, modeling, measurement and other activities where R&D collaboration among industries that use atomization or spraying technology with support from academia and national laboratories could provide significant benefits to U.S. manufacturing.

- **Understanding the physics of fluid flow**, including how energy and momentum of high-velocity gas or water streams affect the break-up of fluid streams to form droplets from materials with a wide range of physical properties, especially high surface tension and high viscosity.

- **Development of advanced physics-based models based on first principles**, which can provide insight into the sensitivity of key variables that affect atomization and spraying processes.
• **Using high performance computing facilities to conduct numerical simulations and modeling** to understand the atomization behavior of liquids at local regions throughout the entire spray pattern.

• **Enabling greater collaboration with suppliers of advanced imaging technologies** to develop improved imaging capabilities that can advance the study of atomization and spraying phenomena, especially in harsh environments.

• **Experimental and computational work to understand how liquid or liquid-solid droplets impact surfaces or semi-solid layers**, for example:
  - Spraying droplets of pesticides that adhere on the leaves of crops
  - Interaction of droplets of gasoline against the cylinder walls of internal combustion engines
  - Application of paint sprays on vehicle body parts
  - Deposition of coatings on glass sheets
  - Application of high-density deposits by thermal spraying of oxidation resistant molten metals and ceramics to coat internal surfaces of jet engines that are exposed to extreme heat
  - Using atomization spray forming to continuously deposit molten or semi-solid metal droplets in layers or pools that rapidly solidify as a coating or near-net billet with a fine grain size.
Current Challenges

To establish the physical property data and standards needed to accelerate the development and implementation of advanced atomization and spraying technology, the research community must address the challenges that follow.

Lack of pedigreed fluid physical property data

There is currently a limited availability of pedigreed physical property data on viscosity and surface tension for liquids and molten metals as a function of temperature, flow rate, and composition. This lack of verified, accessible data hampers the modeling of atomization during primary break-up, steady-state, and transient conditions due to the unknown sensitivities of physical properties on model predictions. Additional physical property data needs include the evaporation rate for pure liquids, solutions, and slurries as a function of temperature; the oxidation rate for molten metals as a function of temperature and composition; and, for atomization of molten metal with a two-fluid nozzle that uses air or an inert gas for atomization of molten metal, the detailed temperature dependent physical property data for pure or mixed inert gases and air.

Lack of in-nozzle and near-nozzle fluid physical property data

The ability to model and characterize regions of dense spray is critical to understanding how fluid instabilities and perturbations affect the break-up of liquid streams as they emerge from the tip of the nozzle. In-nozzle and near-nozzle fluid physical property data is needed to conduct this modeling accurately. In addition, quantification of uncertainty in physical data is also critical to understanding the capability of models to accurately predict atomized droplet characteristics such as size and concentration under actual operating conditions.

Limited understanding of the relationship between standardized nozzle/injector designs and spray distribution

Understanding the impact that nozzle design has on resulting spray of liquids is critical to improving control. Yet, researchers currently do not fully understand the relationship between droplet characteristics and the atomization parameters of standard nozzles. Systematic studies using diagnostic tools on spray patterns from standard nozzles are needed to provide baseline information on droplet size, distribution, shape, density, velocity, and direction.

Inadequate understanding of how powder size and distribution relates to industry standards and end user requirements
Because models predicting atomized powder size and distributions are limited by the lack of physical property data of molten metal alloys, trial and error experimentation is typically used to learn how changes in process parameters affect powder size and characteristics. However, proprietary nozzle designs and atomizing systems developed by producers of atomized powders prevents sharing of best practices and makes it difficult to set consistent standards. In addition, for applications that require powders with specific densities, there is a lack of a clear understanding of what atomized powder characteristics are needed for optimum performance of the final part.

**Lack of methods for consistent powder size measurement**

A round-robin study using laser diffraction to measure particle size on the same powder at a range of laboratories produced different results, indicating that researchers do not yet have a method for measuring powder size consistently (Mingard et al, 2009). There is also currently no industry-accepted method for assessing powder shape for applications or specification for powders for thermal spray.

**Limited measurement tools for and understanding of how atomized powder properties relate to additive manufacturing processes and products**

Current methods for measuring the flow of powders used in additive manufacturing (AM) processes are inadequate. Powder characterization tools generally fail to accurately predict transfer of powders during processing or powder performance in AM applications. This limitation of measurement tools inhibits the ability to fine-tune powders in ways that improve AM process efficiency and product quality. In addition, there are knowledge gaps regarding how powder properties relate to requirements for specific applications. Filling these gaps is critical to the development of improved standard specifications for powders used in AM processes.

**Priority R&D Activities**

The challenges related to the lack of physical property data and standards can be addressed by the R&D activities listed in Figure 7. Priority activities are listed in bold and described in detail below.

**Develop a database of Newtonian/non-Newtonian fluid rheological properties, including nozzle and spray characteristics**

Establishing an accessible database of Newtonian/non-Newtonian fluid rheological and physical property data will ensure that researchers can consistently conduct computational fluid dynamics (CFD) modeling to advance spray technologies and optimize the liquids they use. This database should include data capturing the effects of temperature changes on viscosity, surface tension, and the rate of evaporation or oxidation; characteristics of droplets such as size, distribution, shape, and density; and spray patterns of standard fluids atomized with standard nozzles under typical operating conditions. While pedigreed physical property data from existing handbooks, papers, and other reliable sources may be used initially to populate the database, it will eventually need to be expanded by generating experimental physical property data on new or modified fluids that include a wider atomized spray operating range, such as differing temperatures or pressures.
### P1. Physical Property Data and Standards

<table>
<thead>
<tr>
<th>Activity</th>
<th>Near (0–2 yrs)</th>
<th>Mid (3–4 yrs)</th>
<th>Long (5–10 yrs)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Develop a database of Newtonian/non-Newtonian fluid rheological properties, including nozzle and spray characteristics</td>
<td>●</td>
<td>○</td>
<td>○</td>
</tr>
<tr>
<td>Develop a summary of existing rheological data suitable for use in computational fluid dynamics (CFD) modeling</td>
<td></td>
<td>●</td>
<td></td>
</tr>
<tr>
<td>Create a database of standardized fluid/nozzle/operating conditions and conduct characterization experiments</td>
<td>○</td>
<td>○</td>
<td></td>
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<tr>
<td>Evaluate standardized sprays to evaluate diagnostic equipment and modeling capabilities</td>
<td>○</td>
<td>○</td>
<td></td>
</tr>
<tr>
<td>Extend the fluid property database to include a wider operating range of atomized dense sprays</td>
<td>●</td>
<td>○</td>
<td>●</td>
</tr>
<tr>
<td>Develop a database on thermophysical properties of alloy melts (e.g., surface tension, viscosity, and oxidation rate for process modeling)</td>
<td>○</td>
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<tr>
<td>Develop a database of atomization parameters and powder characteristics to facilitate benchmarking and user-friendly alloy modeling</td>
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<tr>
<td>Perform round-robin testing of powder size across equipment types and measurement procedures</td>
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<tr>
<td>Generate experimental material property data for key alloys by creating a test bed</td>
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<td>Initiate benchmark measurement studies to evaluate variability in characterizing powder quality as a function of process variables</td>
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<td>Survey AM equipment suppliers and powder users to obtain information on needs</td>
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<td>Proactively collaborate with standards organizations to define AM powder specifications</td>
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<td>Initiate a R&amp;D program to develop standard atomized powder measurement methods using round-robin data for the development of particle size, particle size distribution (PSD), and shape measurements</td>
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<td>Define standards for powder characteristics (e.g., flowability and spreadability) that correlate to particle size distribution measurements</td>
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<td>Promote joint powder test programs between AM machine builders and powder producers</td>
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</table>
Develop a database with pedigreed thermophysical properties of alloy melts (e.g., surface tension, viscosity, and oxidation rate for process modeling)

The development of an accessible database of standard alloy melt properties including surface tension, viscosity, density, and oxidation rate as a function of temperature will support researchers' efforts to effectively model atomization during primary break-up, steady-state, and transient conditions. For standard alloys, physical property data could be gathered from existing public sources, while data for new or experimental alloys and the physical properties of melts could be generated by thermophysical evaluations of alloys at research laboratories that have expertise in measurement of physical properties of materials.

Develop a database of atomization parameters and powder characteristics to facilitate benchmarking and user-friendly alloy modeling

A database that contains atomizing data (e.g., pressures, gas-to-metal ratios, powder size, and distribution) would serve as a useful source of data for powder producers to use in benchmarking, as well as a pedigreed source of data for modeling atomization to predict powder characteristics such as size and distribution as a function of atomizing process variables.

In the case of additive manufacturing, a collaborative powder evaluation program between AM machine builders and powder producers should be initiated. The joint testing program would establish an understanding of the relationship of powder size and distribution measurements to measure powder flowability and spreadability measurements and make relevant data available. This can lead to improved AM powder standards and specifications.

Perform round-robin testing of powder size measurements across equipment types and measurement procedures

Information on particle size measurements from different particle size measurement equipment is needed to strengthen researchers' understanding of how to interpret and use resulting measurement data. Round-robin testing of reference powder lots would use laser diffraction particle size measurement equipment from different suppliers. Measurements conducted by the different laboratories would be compared to the powder size results obtained from sieving and metallography.
CASE STUDY: The Importance of Biofuel Physical Properties on the Characteristics of Atomized Droplets

*University of California-Irvine, Combustion Laboratory*

**Challenge**

Interest in biofuels is growing due to a desire to expand the use of renewable energy sources, depletion of fossil fuels, fluctuating prices of petroleum-based fuels, the increased capacity to produce biofuels from agricultural products, and climate change concerns. However, when biofuels are injected into land-based turbine engines, differences in the physical properties of biofuels (e.g., higher viscosity and surface tension compared with conventional diesel fuel, may increase the size of atomized droplets, which can lead to increased NOx emissions. The ability to use biofuels in place of fossil fuels is therefore dependent on understanding the effect that different physical properties have on generating small droplet sizes of atomized fuel to meet air quality standards for fuel combustion.

**Approach**

Researchers at the University of California-Irvine conducted a study to evaluate the potential use of biodiesel fuels in land-based turbine engines by examining how the physical properties of renewable biodiesel fuel blends affect atomized droplet size and spray pattern produced by the air blast atomizer nozzle typically used in gas turbines. The kinematic viscosity and surface tension of B99 biofuel blends were measured and compared to the physical properties of baseline fuels #2 diesel and F76 Navy Distillate (see Figure 1). The approach involved varying the addition of ethanol to biofuel B99 to create a range of viscosities and surface tensions above and below those of the baseline fuel.

An experimental setup with an air-blast nozzle was used to generate atomized droplets under various fuel-to-air ratios. Several diagnostic methods were used to characterize atomized fuel droplets, including a phase Doppler particle analyzer (PDPA) and a laser Doppler velocimeter (LDV), which were used to measure the Sauter mean diameter (SMD) and droplet velocity. Simultaneously, a high-speed camera was used to visualize the fuel breakup of biofuel blends in comparison to the spray patterns of baseline fuels.

**Results/Impact**

As shown in Figure 2, baseline fuels DF2 and F76 had maximum droplet sizes of 32 microns, while biofuel B99 had a maximum SMD droplet size of 42 microns. To study the influence of lower
Roadmap for the Development of Advanced Atomization and Spraying Technologies

viscosity and surface tension on droplet size, two B99-ethanol blends were created by mixing 80% biofuel B99 with 20% ethanol (BE80) or by mixing 60% B99 with 40% ethanol (BE60). The results show that the SMD droplet size decreased as the amount of ethanol increased. With this evidence, researchers were able to determine that blending ethanol with biofuel B99 lowers viscosity and surface tension, which results in a lower average SMD droplet size and makes the biofuel blends potential candidates for use in turbine engines.

Figure 2. SMD distributions for various atomized fuels at a high air pressure drop

References

CASE STUDY: Global Standards for Atomized Powders Used in Additive Manufacturing

Fraunhofer, IFAM

Challenge
Additive manufacturing (AM) has been growing significantly in recent years—in 2015, sales of global AM products and services grew by 25.9% to $5.165 billion.1 As a relatively new application for atomized powders, one of the challenges associated with the rapid growth of AM is the need for universal standards that can be used by global atomized powder alloy producers. Although some AM powder standards are being developed by high-volume aerospace and medical applications—such as titanium alloy medical implants, cobalt-chrome dental copings, and cobalt-chrome aircraft nozzles—most major AM part production companies have created their own different internal guidelines for the use of powders in specific AM machines.2 These different standards have inhibited the worldwide production of AM parts with consistent mechanical properties.

Approach
To address the need for universal powder standards for additive manufacturing, two leading international standards institutions, ISO (International Standardization Organization) and
ASTM International have been actively working to develop and publish AM standards. In 2009, ASTM established an International Committee F42, and in 2011, ISO began Technical Committee TC261. In July of 2013, ASTM and ISO agreed to establish a joint development plan for developing international AM standards that includes nomenclature and data formats, materials and testing.

Results/Impact
Currently the ASTM subcommittee F42.05 on Materials and Process has established four AM standards on powders including Ti-6-4, Ti-6-4 (ELI), IN718, and IN625. There are also three new standards proposed for cobalt-chrome, 316 stainless, and AISi10Mg. In addition, other metal alloy powders used in AM development programs (e.g., 17-4 PH stainless steel, platinum, molybdenum, and tungsten), will need international standards.

Characterization of Powders
In addition to standards that define the chemistry and size of powders that are being used to produce additive manufactured parts, ASTM has established standard ASTM F3049-14, Standard Guide for Characterizing Properties of Metal Powders Used for Additive Manufacturing Processes. Figure 1 illustrates the reason that accepted standardized methods for characterization of powders is important. It is apparent from the photographs that each atomized powder has significantly different flow behavior. The ability of powders to have consistent flow properties is key parameter for using powders in AM processes such as powder bed fusion or directed energy deposition.

References
3. ASTM Subcommittee F42.05 on Materials and Processes, https://www.astm.org/COMMIT/SUBCOMMIT/F4205.htm
Current Challenges

Process models that can efficiently and accurately model spraying and atomization mechanisms are critical to the advancement of atomization and spray technologies. To develop and implement these process models, the research community must address the challenges that follow.

**Limited ability of models to simulate multi-phase flow under transient conditions**

Current atomization models do not completely incorporate first principles of physics, and accurate physical property data is not available. As a result, researchers cannot effectively model multi-phase flow under transient conditions. For example, the characteristics of sprays from injector nozzles could be better predicted by incorporating the effects of temperature on rheological data and underlying theories of fluid break-up mechanisms into advanced models.

**Lack of models that reflect the relationship between internal nozzle geometry, spray, and combustion dynamic interaction**

To improve control over fuel sprays used in combustion engines, it is critical to use models that reflect how the internal nozzle geometry and surface condition affect fluid flow and generation of droplets at the tip of the nozzle. For gas turbines, minor changes to the geometry of the internal passageways or the presence of surface roughness or defects such as a burr can alter the flow of fuel inside the injector and affect the pattern of the atomized droplets and efficiency of combustion.

**Limited understanding of impingement spray dynamics (e.g., sprayed droplets and solid surface interactions)**

Improved models are needed to understand how the droplet size, velocity, and travel distance to the surface affect the desired impingement of atomized sprays on solid surfaces such as coatings, paints, and agriculture sprays. For internal combustion gas engines and diesel engines, avoiding adverse effects of atomized droplet impingement on the cylinder walls is important so as not to reduce engine performance. Models need to account for how differences in density, surface tension, and viscosity affect droplet size, distribution, and velocity, and the angle of impact of atomized fuels.
Lack of readily available analytical and numerical modeling tools for the atomization of molten metals

Current methods have limited ability to provide predictive primary molten metal atomization simulations for powders at a reasonable cost. These models also lack the ability to describe how atomization parameters affect the surface roughness of atomized powders. A better understanding of the molten metal and oxygen reactions at the droplet surface is needed to create improved passivation of films on the solidified powder. Improved models for two-fluid gas atomization that relate momentum and energy transfer are also needed to enable better size control of powders by coupling gas jets with the flowing melt.

Priority R&D Activities

The challenges related to the lack of effective and accurate process modeling can be addressed by the R&D activities listed in Figure 8. Priority activities are listed in bold and described in detail below.

Develop standardized test cases for modeling

Standardized test cases defined by modeling experts can be used to compare predictions from various models and with experimental results. Validating models with standard test cases enables modeling of various types of nozzles to be performed that can make great strides in evaluating specific problems, such as different internal flows within nozzles and their effects on resulting spray patterns.

Develop advanced theoretical models to understand the physics of atomization

The development of comprehensive models based on theory and first principles of physics that incorporate the hydrodynamic and aerodynamic factors involved during disintegration of fuels under typical atomization conditions is essential to enable the prediction of droplet size and distribution. For turbine engines aiming to achieve low emissions, the ability to also model the symmetry of the mass flux of fuel distribution within turbine engines is as important as the modeling drop size. For example, the lack of a uniform spray pattern due to an inhomogeneous mixture of fuel droplets and air in turbine combustion zones can increase the amount of emissions. Other factors that affect the uniformity of fuel spray patterns from nozzles and could be modeled include poor surface finish, roughness of internal channels, plugged flow passages, and lack of symmetry of passageways, which can lead to blockage of atomizer nozzles due to carbon deposition.

Develop physics-based models that can predict the impacts of multi-phase flows with phase changes

The use of physics-based ensemble spray models for prediction and verification of nozzle performance can aid the development and optimization of spraying applications. Incorporating the ability to model multiphase flows that account for differences in fluid viscosity, surface tension, and the transition from sharp to diffuse interfaces at the droplet surface is important for accurately modeling two-fluid atomization processes. One potential use of these advanced physics-based models is investigating supercritical diesel fuel-injection systems, which by raising the temperature of diesel fuel with supercritical injection produces fine
vapor-like droplets that mix more evenly with intake air to burn rapidly with up to 80% reduction in engine emissions.

**Develop an adaptable, open-source model for molten metal atomization processes**

The development of a universal model for predicting atomized powder size based on open-source codes would aid not only in developing a better understanding of breakup mechanisms, but also in improving nozzle design. Ideally, the model would be developed by a collaborative group of representatives from industry and academia to help ensure that it is practical and easy-to-use, has the ability to model a variety of atomization processes and types of nozzles, and could potentially support real-time sensor feedback and process control. Data from imaging atomizing nozzles and sensors could be used to refine and validate the model predictions.
CASE STUDY: Hierarchy of Computational Fluid Dynamics Models

U.S. Department of Energy

Challenge
The automotive industry is under increasing pressure to develop more fuel-efficient engines with reduced emissions. Modeling the fine details of complex spray patterns can aid automotive engineers in the development of improved internal combustion and diesel engines by increasing understanding of the primary and secondary breakup mechanisms as jets of fuels are atomized (see Figure 1). Yet, it was unclear exactly how advanced simulation models could be best deployed to help accelerate research specifically on improving fuel economy of internal combustion engines.

Approach
To identify applications where modeling and numerical simulation using supercomputing could help reduce the time required by the automotive industry to develop cleaner, more fuel-efficient engines with 30 to 50% greater fuel economy, the U.S. Department of Energy (DOE) Office of Science and the Energy Efficiency & Renewable Energy sponsored a workshop on predictive simulation. Sixty experts in the engine combustion field from industry, academia, and national laboratories met to identify challenging problems where advanced simulation could reduce the development cycle time for internal combustion engines. These experts recognized that computational fluid dynamics (CFD) models and numerical algorithms are essential to improving the understanding of the fuel spray pattern behavior. Figure 2 illustrates the various levels of image fidelity that can be generated with various types of hierarchical models.

Depending on the research objective, details of turbulence in the experimental spray pattern (Figure 2a) can also be generated by modeling using direct numerical simulation for simple flows; however, the computational requirements for DNS modeling can be very high. As shown in Figure 2b, high fidelity large eddy simulation (LES) modeling, using dense computational meshes, is capable of creating detailed turbulent flow patterns. In contrast,
Figure 2c shows a lower fidelity simulation that was generated with a coarser grid computational fluid dynamics model. The image with the lowest level of flow pattern details is Figure 2d. The image was generated by a Reynolds averaged Navier-Stokes (RANS) calculation, which is the least computationally expensive method.

Impact
There are significant benefits to using advanced CFD simulation models to reduce the time and cost to develop more efficient engines. For example, Cummins has demonstrated the ability to design a 6.7-liter diesel engine based solely on computer modeling, which reduced development time and cost by 10%.1 Engine testing was done only to confirm predictions from models of improved mileage and emission levels. DOE notes that other industries have reduced product development cycles by one-third through the use of computer-based simulation. It is therefore essential that advanced CFD models be applied as widely as possible to improve the design of atomization and spraying nozzles to optimize process efficiency.

References
Current Challenges

Numerical simulation and high-fidelity, physics-based models provide detail on the mechanisms that influence the break-up of fluids that are critical to the advancement of atomization and spraying modeling and process improvements. To improve and implement advanced simulation and modeling, the research community must address the challenges that follow.

Lack of integrated multiscale, multiphysics, high-fidelity spray models for simulation of atomized fluids

Currently, there are not many physics-based models capable of predicting droplet size based on theory and first principles. This gap limits the ability to simulate atomized fluids, including fuels for combustion, water and water-base solutions (including the effect of surfactants), and electrostatic spraying, among others. Advanced modeling capabilities that can simulate small-scale details would be beneficial to understand the atomization behavior of a wide variety of fluids and validate experimental trials of different types of nozzle geometries.

Insufficient accessibility to high-performance computing systems

Complex numerical simulations of fluid behavior based on advanced physics-based models requires the use of high-performance computing (HPC) resources. The current use of HPC systems for modeling fluid atomization is limited by several barriers, including the prohibitively high cost to access an HPC system, the limited availability of experienced personnel capable of operating HPC systems, and the low priority given to modeling sprays versus other uses of HPC resources.

Inadequate ability to predict the impacts of internal flows, geometries, and atomizer nozzle design flaws

Primary atomization and secondary droplet break-up is greatly impacted by a range of variables, including internal flows, geometries, and design flaws in atomizer nozzles. While these variables can greatly influence the resulting break-up, there are currently not many methods for predicting and measuring the impacts. Advanced high-fidelity models would enhance the ability to simulate the flow of fluids inside nozzles with different geometries and provide the capability to model the effects of small internal defects of nozzle channels nozzles on the characteristics of atomized droplets.

Priority R&D Activities

The challenges to conducting modeling and numerical simulations of atomization and spray processes can be addressed by the R&D activities
listed in Figure 9. Priority activities are listed in bold and described in detail below.

**Conduct engineering-level modeling of the internal injector and spray patterns**

Modeling the internal injector flow and the impact on the downstream spray can provide information that will enable engineers to design more efficient injectors for atomization of fuel. Modeling should encompass the impact of internal swirl on interfacial dynamics, the exit spray angle, and drop size. Simulation of flash boiling and effervescent injector flow are other phenomena that would benefit from improved modeling approaches. Modeling results can “close the loop” on understanding the relationships among injector design, the spray pattern, droplet size, and combustion efficiency.

**Use direct numerical simulation (DNS) on test case injectors to improve understanding of near nozzle/primary atomization of fluids and aid development of new diagnostic techniques**

Collaboration among industries and the research communities that are interested in modeling atomization of injector nozzles is a pathway to advance the understanding and improve performance of nozzles in applications that require precise control of sprayed droplet characteristics. Initially the group could select a few benchmark injectors to extensively study using numerical simulation. Predictions from modeling can be compared to data obtained from experimental evaluations using advanced diagnostics and imaging equipment. Detailed studies on benchmark injectors using mutually defined operating conditions, can provide a better understanding of the behavior of atomized sprays that are relevant to industrial use in jet engine and land-based turbines, internal combustion engines and other high performance applications. Furthermore, the modeling group could focus on selecting unit problems for DNS modeling of individual droplets and entire spray patterns that will expand understanding of underlying physics at steady-state and transient flows over a range of Weber numbers.

**Conduct large eddy simulation (LES) of primary atomization with DNS and low-fidelity approaches**

LES is widely applicable for stochastic simulation of turbulent liquid jet flows (Chigier et al. 2011; Gorokhovski and Herrmann 2008; Herrmann 2011; Arizona State University 2014). For example, a LES subgrid model has been used to study and predict the phase interface dynamics of turbulent liquid/gas flows, leading to optimization of injector design (Arizona State University 2014). There is also need to use lower-fidelity reduced-order models (ROMs) that offer the potential for near real-time analysis of sprays. Due to mathematical approximations, ROMs can be used to speed-up computation time, but building ROMs can be expensive and may lack robustness because the models may need to be rebuilt to accommodate changes in modeling parameters. Use of ROMs in conjunction with LES modeling can help to ensure reduced-order models provide reliable predictions of fluid atomization behavior while providing the faster computational advantages of low-fidelity approaches.

**Conduct computational fluid dynamics (CFD) modeling of two-fluid atomization nozzles to understand the effect of process parameters on fluid flow and droplet characteristics**

Computational fluid dynamic (CFD) modeling is an effective tool to understand the complex
behavior of fluids under a wide range of operating conditions. For modeling the interaction of liquids and gases, CFD modeling has been used to study the internal flow of fluids inside spray nozzles as well as the mixing of gas and liquids in two-fluid nozzles (Spraying Systems Co. 2009). For atomization of molten metals, CFD modeling has also been used to study the effect of gas pressure on recirculation patterns and location of stagnation points downstream of high pressure atomization nozzles (Ting and Anderson 2004). Continuing to develop and apply advanced CFD-based models can provide greater understanding and control of two-fluid atomization processes used for generation of fine droplets of liquids, fuels and molten metals.

Figure 9. R&D Activities for Modeling and Numerical Simulations

<table>
<thead>
<tr>
<th>Key:</th>
<th>Liquid Spray</th>
<th>Molten Metal / Melt Atomization</th>
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<tbody>
<tr>
<td></td>
<td>Near (0–2 yrs)</td>
<td>Mid (3–4 yrs)</td>
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**P3. Modeling and Numerical Simulations**

- Conduct engineering-level modeling of the internal injector and spray patterns
- Use direct numerical simulation (DNS) on test case injectors to improve understanding of near nozzle/primary atomization of fluids and aid development of new diagnostic techniques
- Establish an atomization modeling and simulation summer “boot camp”
- Improve access to high performance government computers and resources for spray research by generating justification for modeling of sprays
- Evaluate empirical-based numeric methods for improved understanding of the impact of spray process controls, internal nozzle geometry, regression on changes on spray patterns
- Define unit problems for direct numerical simulation (DNS) modeling of individual droplets and entire spray patterns that expand understanding of underlying physics at steady-state and transient flows over a range of Weber numbers
- Conduct large eddy simulation (LES) of primary atomization with DNS and low-fidelity approaches
- Recommend modeling approaches based on different types of atomizer nozzles
- Conduct computational fluid dynamics (CFD) modeling of two-fluid atomization nozzles to understand the effect of process parameters on fluid flow and droplet characteristics
CASE STUDY: Hierarchy of Computational Fluid Dynamics Models

U.S. Department of Energy

Challenge
For the past several years, General Electric has been working on developing the capability to manufacture fuel nozzles for jet engines by using 3D printing and improving the nozzle design to improve fuel efficiency. In July 2016, GE Aviation introduced into airline service its first additive manufactured jet engine component—complex fuel nozzle interiors—with the LEAP jet engine.1,2 The LEAP jet engine was developed by CFM International, a joint venture between France’s Snecma (Safran) and GE Aviation. More than 11,000 LEAP engines are on order with up to 20 fuel nozzles in each engine. Annual production of additive manufactured fuel nozzles is planned to ramp up to more than 40,000 nozzles by 2020.

In addition to development of the manufacturing capability to produce 3D-printed fuel nozzles, extensive modeling of fuel nozzles by numerical simulation was performed using high performance super computers.3 The objective was to use supercomputers to optimize the design of 3D printed injectors to improve the dispersion of fuel droplets. Injectors atomize liquid jet fuel into fine droplets that are sprayed into the combustion chamber and where they burn to generate energy for propulsion. The fuel injector is one of the most challenging parts to design and very expensive to manufacture due to its intricate geometry.

Approach
To build a better jet engines, GE engineers are utilizing one of the world’s most powerful computers, named Sierra, which is located at California’s Lawrence Livermore National Laboratory and a second supercomputer, named Titan, which is located at Oak Ridge National Laboratory. To optimize the design of the fuel injector, engineers in the Computational Combustion Lab at GE Global Research teamed up with researchers from Arizona State and Cornell universities to use the Titan and Sierra supercomputers to study the behavior of fluid flow and droplet formation. Researchers used between 500,000 and 1 million CPU hours of time to simulate atomization of the liquid jet fuel and spray. Simulation with supercomputers enables...
Approach
High-fidelity numerical simulations of fuel injectors with supercomputers increases understanding of the physics of fluids and how air and droplets of fuels mix and burn. Small changes to fuel nozzle geometry can lead to significant improvements in engine performance, which results in more powerful engines that consume less fuel and have lower emissions. The use of 3D printed fuel injectors has helped to make the LEAP engine 15 percent more fuel efficient with an equivalent reduction in CO2 emissions compared to previous engines built by CFM International. Simulations on fluid behavior high performance supercomputers could also yield new insights beyond jet engines and improve injectors used in locomotives and land-based gas turbines.

References
2. GE Plans to Invest $1.4B to Acquire Additive Manufacturing Companies Arcam and SLM; September 6, 2016 – GE News Release http://www.geaviation.com/additive/
Current Challenges

The ability to characterize detailed features of atomized droplets and spray patterns is an important tool for understanding atomization processes. Using advanced diagnostic equipment, such as Doppler particle analyzers and imaging techniques such as high-speed cameras, x-ray or schlieren diffraction imaging enables researchers to directly observe and measure droplet characteristics (e.g., size, shape, distribution, velocity) in response to atomization and spray process variations. To effectively broaden the use of advanced diagnostic equipment and measurement techniques for analysis of spray and atomization processes, the research community must address the challenges below.

Need for improved accuracy of dense spray measurement techniques that can be used for computational fluid dynamics (CFD) model validation

Improved imaging techniques are needed to obtain droplet size, shape, and velocity measurements of optically dense sprays as well as the entire spray pattern. Measurements and imaging at high speeds of local concentrations and density gradients of droplets in dense sprays close to nozzle exit are particularly challenging, especially for fuels and molten metals due to high temperatures that exist in combustion or atomizing chambers. For imaging atomization of liquids that simulate Jet A fuel sprays, measuring fluorescent particle density and particle velocity in liquids that are equivalent to Jet A fluid in viscosity and surface tension is particularly challenging. Standardized methods for processing images of spray ligaments, fragments, and droplets are needed to enable comparison of imaging results.

Limited access to advanced diagnostic and imaging equipment for characterizing atomized droplets and spray patterns

Currently, the high cost of diagnostic and imaging equipment and specialized training required to operate the measurement equipment inhibits many companies from using these valuable methods to better understand fluid behavior during atomization. Lower cost, easy-to-use equipment will enable researchers to increase the use of diagnostic and imaging equipment in their experimental work, which ultimately will improve atomization and spray processes.
Priority R&D Activities

The challenges to using advanced imaging techniques to measure atomization and spray processes can be addressed by the R&D activities listed in Figure 10. Priority activities are listed in bold and described in detail below.

Conduct experimental evaluations of spray patterns from standardized test case nozzles with advanced diagnostic equipment

Characterization of standard nozzles and spray patterns with advanced diagnostic and imaging techniques will provide baseline information on standard nozzles. The use of advanced diagnostic equipment to characterize atomized sprays from standard nozzles will provide an understanding of the capabilities of imaging tools. Many types of diagnostic equipment and imaging methods (Fansler and Parrish, 2015), (Bachalo, 2000), (TSI, 2016), Artium Technologies, 2016) can be used to obtain detailed measurements of sprays, including optical imaging with back-illumination and Schlieren techniques, phase Doppler particle analyzer (PDPA) with laser Doppler velocimeter (LVD), particle image velocimetry (PIV), phase Doppler anemometry (PDA), high-speed imaging cameras or x-ray imaging. A priority research activity is to simultaneously use multiple imaging techniques to characterize various types of spray nozzles, e.g. pressure swirl air blast, hydraulic and other standard nozzles to compare and contrast experimental results of droplet size, distribution, shape, density, velocity and direction.

Today’s diagnostic equipment and imaging techniques used to characterize atomized sprays requires significant expertise to operate. Modifying commercial diagnostic equipment to be more user friendly could significantly expand the use and potentially lower the cost of diagnostic equipment that can be used to characterize droplets and spray patterns for a wider range of industrial applications.

Characterize dense spray patterns by combining measurement techniques (e.g., digital in-line holography, phase Doppler anemometry (PDA), ballistic imaging, and other interferometric techniques)

For investigating regions of dense sprays, key parameters of sprays to be measured need to be defined to determine which techniques are most applicable. By mapping the operational envelope of various diagnostic techniques and comparing outputs from different imaging equipment, the best approaches for imaging droplets and spray patterns can be defined compared to traditional optical density measurements. It is important to fully characterize dense sprays and correlate discrete spray images with predictions from advanced models. For specialized studies on understanding fluid flow within nozzles or the formation of droplets after atomization, micro-particles or index matching liquids may be utilized. There is also a need to identify surrogate fluids to simulate the atomization behavior of jet fuels and other hazardous fluids to make imaging and diagnostics evaluations easier and less hazardous.
## P4. Diagnostic Methods

<table>
<thead>
<tr>
<th>Activity</th>
<th>Near (0–2 yrs)</th>
<th>Mid (3–4 yrs)</th>
<th>Long (5–10 yrs)</th>
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<tbody>
<tr>
<td>Conduct experimental evaluations of spray patterns from standardized test case nozzles with advanced diagnostic equipment</td>
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<tr>
<td>Characterize dense spray patterns by combining measurement techniques (e.g., digital in-line holography, phase Doppler anemometry [PDA], ballistic imaging, and other interferometric techniques)</td>
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<tr>
<td>Map operational envelope of optical diagnostics (vis-a-vis optical density)</td>
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<tr>
<td>Utilize micro particles and index matching liquids to map atomizer internal flows</td>
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<tr>
<td>Modify current commercial advanced diagnostic equipment to be user friendly</td>
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<td>●</td>
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<tr>
<td>Identify surrogate fluids for jet fuels and other hazardous fluids to make diagnostics and testing easier</td>
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</tr>
<tr>
<td>Identify best approaches for imaging droplets and spray patterns by comparing outputs from different imaging equipment</td>
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<td>●</td>
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<tr>
<td>Correlate discrete spray images with predictions from advanced models</td>
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<td>●</td>
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<tr>
<td>Fully characterize dense sprays experimentally and computationally</td>
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</table>
P5 REAL-TIME SENSORS

Current Challenges

There are several measurement techniques based on laser diffraction that industry can employ to obtain real-time data on the size and distribution of liquid droplets or solid particles for use in adjusting atomization and spraying parameters. Sensors that can detect changes in droplet characteristics in real time can also be used to identify issues such as nozzle wear or clogging that affect steady-state atomization of liquids or molten metals. To enable the broader use of advanced real-time sensors for applications, the research community must address the challenges that follow.

Limited ability to control spray droplet sizes on demand

Liquid spray systems that use hydraulic or air-assisted nozzles typically produce a fixed droplet size and distribution that is difficult to adjust during atomization. In many commercial and industrial spray processes, the ability to adjust the droplet size and distribution during atomization could enable the mass flux and spray pattern to be tailored to changes needed by the application. Enabling this real-time control of online actuators requires feedback from sensors that can actively monitor sprayed droplet size and spray patterns. For example, sensors that can detect changes in droplet size and velocity during the chemical spraying of crops can be used to optimize the amount of the chemical spray applied relative to the ability of the droplets to adhere and uniformly coat the surface of the leaves. To realize this level of control, robust sensors that can provide reliable, continuous feedback need to be developed and implemented into spray processes.

Lack of widespread adoption of real-time, atomized powder characterization methods as in-line process sensors to ensure powders consistently meet specifications

Widespread adoption of robust, real-time, and affordable sensors and in-situ monitoring techniques is needed to measure atomized powder particle size. Active sensing and control of major atomization parameters can enable powder producers to maintain steady-state powder size by ensuring the atomizing process remains in a state of statistical process control. In-line devices that provide real-time particle size data are commercially available today, but understanding the capabilities and limitations of these devices and how they can be used as real-time sensors to enable process control remains incomplete.
Priority R&D Activities

Advanced sensor capabilities have significant potential to increase the ability to control the consistency of atomization and spraying processes. Although current sensors have the ability to measure key in-situ droplet or particle parameters—such as temperature, size, velocity, and shape—challenges remain before the capabilities of sensors are linked to actuators to achieve real-time control of spray or atomization processes. The challenges to implementing advanced measurement and sensing methods into atomization and spraying processes can be addressed by the R&D activities listed in Figure 11. Priority activities are listed in bold and described in detail below.

Apply existing or develop new diagnostic equipment for sensors to monitor and control spray processes

For study of liquid sprays, a number of diagnostic methods are used to characterize droplet size, velocities, and spray patterns during short time experimental tests that are conducted using controlled process parameters. For continuous monitoring and control of sprays for industry applications, commercial systems based on laser diffraction are available, such as phase Doppler particle analysis (PDPA) and particle image velocimetry (PIV). A survey of laser-based systems that have the ability to continuously monitor spray patterns and provide timely information to enable control of the fluid flow control is needed. For some sprays, existing diagnostic or new diagnostic equipment may need to be developed for use as real-time sensors.

Perform a broad-based gap analysis to determine sensor needs by industry versus available sensor technologies for process control

Real-time sensors are required during continuous atomization of molten metal over many hours to ensure variations of processing parameters—such as molten metal temperature; molten metal, gas or water flow rates; or erosion of nozzles—do not affect powder size, distribution or shape. Many sensors that can monitor process parameters—such as infrared temperature measurement instruments and flow rate gauges—already exist, although they may have varying levels of accuracy, reliability, and performance. Conducting a rigorous survey of powder producer measurement needs is required to determine where gaps exist between sensor needs and available sensor technologies. This information should be benchmarked with sensor technologies available in other process manufacturing industries to identify opportunities for improving powder producers to measure temperature, gas and water flow, and particulate opacity.

Develop and test robust in-situ sensors and production process control actuators

As limitations in process control sensors are collectively identified, powder producers should work with instrument suppliers to specify, design, build, and test prototype sensors that are robust and can withstand exposure to the atomization or spraying environments. For example, the particle size produced during atomization of molten metal is a function of the flow rate and temperature of molten metal. Thermocouples typically contained within ceramic protection tubes are immersed in the molten metal pool to measure metal temperature. For gas or water atomized powder production, pressure gauges are used to measure gas or water pressure.
Measurement of flow rate of molten metal by eddy current or other non-contact methods could be beneficial (Ridder 2002).

As limitations in process control sensors are collectively identified, powder producers should work with instrument suppliers to specify, design, build, and test prototype sensors that are robust and can withstand exposure to atomization or spraying environments. Currently, sensors primarily use physical contact to measure flow rate and temperature of molten metal (e.g., immersed thermocouples), as well as gas or water pressure (e.g., pressure gauges). Ideally, sensors that use non-contact methods should be leveraged as well. Examples include measurement of flow rate of molten metal by eddy current (Ridder 2002) or laser-based techniques, such as laser diffraction (Malvern 2016) or phase Doppler anemometry (PDA) (Dantec Dynamics 2016); these techniques can be used to obtain in-situ measurements of droplet or powder size and velocity for atomized powders. Sensors used in other industries that require measurement of molten particles could also be applied, such as the instruments currently used in the thermal spray industry reviewed by Fauchais & Vardelle 2010 (Tecnar Automation 2016, Oseir Ltd. 2016).

<table>
<thead>
<tr>
<th>P5. Real-Time Sensors</th>
<th>Near (0–2 yrs)</th>
<th>Mid (3–4 yrs)</th>
<th>Long (5–10 yrs)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Apply existing or develop new diagnostic equipment for sensors to monitor and control spray processes</td>
<td>✔️</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Use advanced sensors to obtain high quality/reliable data at high pressures and temperatures for CFD validation</td>
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<td>✔️</td>
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<tr>
<td>Apply mass-based (x-ray) diagnostic techniques to evaluate spray patterns near the nozzle exit and in the dense spray core</td>
<td></td>
<td>✔️</td>
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<tr>
<td>Conduct a survey of diagnostic tools to understand the limits and capabilities for different applications, e.g., internal/external fluid flow and spray patterns.</td>
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<td></td>
<td>✔️</td>
</tr>
<tr>
<td>Perform a broad-based gap analysis study to determine sensor needs by industry versus available sensor technologies for process control</td>
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<td>✔️</td>
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</tr>
<tr>
<td>Develop and test robust in-situ sensors and production process control actuators</td>
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<td></td>
<td>✔️</td>
</tr>
<tr>
<td>Develop technologies for in-situ analysis of oxide inclusions and other impurities in melt or powders</td>
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</tbody>
</table>
Current Challenges

Access to facilities to conduct research on sprays of fuels, liquids, and atomized powders is vital to advancing industrial and commercial applications. For research on liquids and fuels, several U.S. universities and national laboratories have experimental, diagnostic, and modeling capabilities to conduct research on sprays. For example, to study atomization of fuel, laboratories at the University of California-Irvine, University of Wisconsin, and Sandia National Laboratories have the experimental capabilities to study combustion. These capabilities complement the significant testing facilities that exist in industry, which are used for proprietary R&D. For example, automotive manufacturers have capabilities to conduct testing of fuel injectors for internal combustion and diesel engines to study the generation of emissions under actual conditions. Companies that produce jet engines and land-based turbines have facilities to conduct full-scale testing of turbines.

In contrast, few such facilities are available for studying atomization of molten metals in the United States. There are some; for many years, Ames National Laboratory in conjunction with Iowa State University has conducted research on atomization. However, facilities that companies can use to conduct atomization trials have been limited. Further, industrial powder producers have limited ability to conduct collaborative research due to the proprietary nature of atomizing nozzles and injectors. Powder producers need to understand how atomization processes affect powder size and distribution, but generally do not have facilities needed to conduct experimental trials under controlled parameters and with diagnostic equipment that can image and measure important atomization characteristics. In addition, the high cost and long preparation time for atomizer runs limits the total number of experiments that can be conducted on large-scale production atomizers. For atomization of molten metals, the research challenges described below could be addressed with an accessible test facility equipped with state-of-the-art diagnostic equipment.

Lack of understanding of key processing variables that control atomized powder quality

The lack of an accessible atomizing test facility hinders the ability of companies to perform controlled experiments to investigate relative sensitivity of process variables. Such work could also help powder producers learn how to limit powder impurities such as oxides, refractories, or other contaminants that are created during atomization of molten metal.

Limited ability to atomize desired particle size and distribution

Today, powder producers cannot obtain a desired size powder size and size distribution
range. Specifically there is a need to control \( d_{50} \) and the standard deviation of atomized powder size that is necessary to meet customer specifications without post-atomization screening of powders. Such screening adds cost, time, and waste to metal powder production that could be avoided with improved ability to control powder size and distribution directly via the atomization process.

**Lack of cost-efficient atomization methods for production of fine powders**

A number of applications, such as metal injection molding, metallic pigments for paints, and some types of additive manufacturing require fine atomized powders of less than 50 microns. Producing such powders is technically demanding and costly, which may limit the commercial growth of specific applications. Thus, innovative cost-effective atomization processing needs to be explored to satisfy the growing markets for fine powders. A pilot-scale atomization facility equipped with state-of-the-art diagnostic equipment and trained operators that could be accessible for industrial research trials would be a valuable asset to enable research on producing fine powders.

**Priority R&D Activities**

The challenges to developing new experimental testing techniques and atomization-focused facilities for industry to use can be addressed by the R&D activities listed in Figure 12. Priority activities are listed in bold and described in detail below.

**Conduct experimental simulations using transparent nozzles to study effects of nozzle geometry, cone angle, internal and ambient pressure, and rheology of fluids on droplet size and dispersion**

Collaborative experiments using transparent nozzles will build fundamental understanding of the effect of nozzle geometry and spray parameters on generation of droplets. Conducting spray sensitivity studies at a testing facility with advanced spray diagnostic equipment will allow researchers to better understand the effects of nozzle geometry, fluid properties, and spray conditions on the spray pattern and droplet size and distribution under steady-state and transient conditions. Other studies that would benefit from collaborative work include examination of the effects of initial disturbance amplitude on jet stability and droplet breakup density near the exit of injectors and a series of round-robin spray tests on nozzles to establish standard deviations and improve collective interpretation of data.

**Establish a user facility for collaborative atomization projects focused on development of equipment and training in PM/AM**

An atomizing facility that is accessible to companies and equipment suppliers can be a valuable test site for evaluation of diagnostic systems, types of nozzles, nozzle materials, atomizing process equipment, sensors and actuators for controls. The atomizer facility would enable research studies to quantify the sensitivity of atomizing parameters on powder size, distribution, and shape and explore new, more efficient, cost-effective, pre-competitive atomizing methods to reduce gas consumption. The atomizer could be used for pilot-scale runs of experimental powders that are used in pressing and sintering, metal injection molding, additive manufacturing, thermal spraying, and cold spraying.

**Develop and launch cross-industry atomization training programs**
The current workforce has only limited trained personnel with direct experience with molten metal and atomizing. As demand for atomization grows, an accessible, experimental atomizer facility could be used to train new operators, technicians, and engineers while also being used for experimental work.

Conduct collaborative studies on step-change (disruptive) process control technologies to adjust particle size and increase yield of atomized powders

Conducting collaborative atomization experiments in a test facility can develop insight into approaches to increase the yield of atomized powder within a desired distribution. The test atomizer can be used to explore innovative processing methods to generate powders with powder sizes and distributions.

<table>
<thead>
<tr>
<th>P6. Experimental Test Facilities</th>
<th>Near (0–2 yrs)</th>
<th>Mid (3–4 yrs)</th>
<th>Long (5–10 yrs)</th>
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<tbody>
<tr>
<td>Conduct experimental simulations using transparent nozzles to study effects of nozzle geometry, cone angle, internal and ambient pressure, and rheology of fluids on droplet size and dispersion</td>
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<tr>
<td>Conduct experiments to quantify the uncertainty of droplet size and spray pattern measurements within the capability of diagnostic equipment</td>
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<tr>
<td>Perform more experiments on internal combustion or turbine engine injectors to study the generation of emissions under actual conditions</td>
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<tr>
<td>Plan and conduct round-robin spray tests on nozzles to establish standard deviations and improve interpretation of data.</td>
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<tr>
<td>Conduct high temporal and spatial resolution studies of injectors near the exit to understand the effects of initial disturbance amplitude on jet stability and droplet breakup density</td>
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<tr>
<td>Perform spray parameter sensitivity studies to understand how the nozzle geometry, fluid properties and spray conditions affect the spray pattern under steady-state and transient conditions</td>
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</tr>
<tr>
<td>Establish a user facility for collaborative atomization projects focused on development of equipment and training in PM/AM</td>
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<td></td>
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<tr>
<td>Develop and launch cross-industry atomization training programs</td>
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<td>○</td>
</tr>
<tr>
<td>Define a strategy to develop more efficient cost-effective, pre-competitive new atomizing methods</td>
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</tr>
<tr>
<td>Perform research to identify and quantify effects of parameters on water/ gas atomization</td>
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<td></td>
</tr>
<tr>
<td>Conduct collaborative studies on step-change (disruptive) process control technologies to adjust particle size and increase yield of atomized powders</td>
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</tr>
</tbody>
</table>

Figure 12. R&D Activities for Experimental Test Facilities

Key: Liquid Spray  Molten Metal / Melt Atomization
and characteristics that are required by specific applications. Powder producers can benefit by applying knowledge from collaborative experimental studies to maximize the yield of desired powder sizes.

CASE STUDY: Testing Facilities for Atomization Experiments

U.S. Department of Energy, Ames Laboratory and University of California - Irvine

Challenge

Producers of atomized powders have a need to understand how atomization processes affect powder size, distribution, and shape, but generally they do not have the ability to conduct sequential experimental trials to explore a wide range of atomizing parameters. Furthermore, commercial powder atomizers are typically not equipped with real-time, advanced diagnostic equipment such as laser-based particle size and velocity measurement systems and high speed cameras that can capture in-situ optical images of atomized droplets. Additional factors that limit the number of experiments that can be conducted on large-scale production atomizers is the high cost and long preparation time to conduct experimental atomizer trials.

Approach

An atomizing facility that is available for research on atomized powders can accelerate development of commercial applications of new atomized alloy powder products and sprayed deposits of metallic and polymer powders, along with, potentially, glass and ceramic powders. Atomizing facilities that are available to users can encourage collaboration between companies, universities, and national laboratories. Access to atomizer facilities equipped with state-of-the-art imaging equipment and sensors can enable fundamental research studies to be conducted to obtain a better understanding of the effect of atomizing parameters on powder size, distribution, and shape. Another benefit of atomizing facilities that are accessible to the metal powder industry is the ability to collaborate with highly qualified and knowledgeable scientists and engineers.

Currently, in the United States, there are only a few facilities available to industry for research on atomization of molten metals. One atomization facility is operated by the U.S. Department of Energy, Ames Laboratory (with support from the Ames Materials Preparation Center), located in Ames, Iowa. Another atomizer is located at The University of California in Irvine, California. Descriptions of these atomizing facilities are given below.

Ames Laboratory

The Ames Laboratory has two unique high-pressure gas atomization systems. A lab-scale gas atomizer with a 5 kg melt capacity is available for experimental trials, while a pilot-scale gas atomizer (PSGA) can produce heats of 30 kg. Both atomizers can produce powders of most metals and alloys of reactive metals including Al, Ti and Mg, as well as atomized powders of special alloys that contain rare earth elements. The atomizers also have novel (patented) passivation capabilities that allow for safe production and handling of fine reactive powders. For titanium alloys, a state-of-the-art melting and special superheating module for close-coupled gas atomization and fine powder production system has been developed. The atomization facility also has the capability to record gas-only schlieren imaging of experimental nozzles and full atomization trials on high-speed video and single image cameras. Examples of research conducted using the atomizing facilities are discussed in several papers and in an Ames Laboratory newsletter.
UC-Irvine Atomization Facilities
The University of California-Irvine, has two atomizers for conducting research on high pressure, gas atomization and spray deposition of molten metals. The melting furnaces are powered by 50 to 100 kW vacuum induction generators, which can heat melts at temperatures up to 1900°C. Atomization chambers are typically evacuated to remove oxygen gas and backfilled with inert gases such as nitrogen or argon to minimize oxidation of molten metal. Many types of metallic powders have been produced, including aluminum and magnesium alloys, steels, superalloys, high entropy alloys, and metal-matrix composites. The atomizing units are equipped with droplet diagnostic capabilities including a phase Doppler particle analyzer (PDPA) for in-situ measurements of molten metal droplet size and velocity and an Insitec ensemble particle concentration and size (EPCS) system, which provides in-situ measurements of sprayed metal droplets based on laser diffraction. A high-speed camera recording system is also available to capture in-situ images of molten metal droplets and the spray pattern. Examples of research conducted using the atomizing facilities are discussed in several papers.6,7

Impact
The availability of spraying or atomization facilities can provide significant benefits to companies that do not have experimental testing facilities that are equipped with advanced, in-situ diagnostic capabilities, which can provide quantitative data on atomized droplet characteristics. The ability to generate information on droplet size, distribution, concentration, and velocity can lead to development of new and improved atomized powder products, advanced diagnostic equipment and longer life materials for nozzles that are resistant to molten metal. Examples of collaborative research are pre-competitive studies on more efficient atomizing methods to reduce gas consumption in close-coupled atomizer nozzles and characterization of atomizing nozzles using state-of-the art diagnostic or imaging techniques to enable producers of diagnostic equipment to evaluate the performance of their equipment under various atomization conditions. The atomizing facilities can also produce small quantities of experimental alloy powders that can be used in powder metal applications such as pressing and sintering, metal injection molding, additive manufacturing, thermal spraying, and cold spraying.

References
Current Challenges

Demonstrating the ability to produce desired droplet or powder characteristics via improved control of atomization or spraying processes during sustained, full-scale operating conditions is critical to impacting industry growth. To enable this real-world success, the research community must address the challenges that follow.

Limited ability to control spray process for on-demand droplet size

Most spray systems lack the ability to adjust the sprayed droplets in real time in response to changing conditions in the spray environment. For example, the size of droplets containing pesticides when spraying crops could be altered in response to changes in the wind velocity to minimize drift of the droplets that are entrained in moving air. The ability to adjust droplet size on-demand for application of paints or coatings can be an advantage, when the viscosity of the paint or coating changes due to temperature or settling of components. In the future, the ability to produce low-cost spray systems that can produce single droplet sprays at high mass flux volumes with uniform deposits could enable new spray applications to become competitive.

Sprays for on-demand cooling applications

Sprays are used for cooling in many manufacturing applications, but the precision of spray-based cooling processes is limited. Researchers lack a complete understanding of spray nozzle and spray characteristics that influence cooling. Armed with such knowledge, specialized cooling applications could employ on-demand adjustment of droplet size and mass flux to respond to changing needs for controlling the amount of in-situ cooling.

Need for improved fuel injectors with discrete jet atomization

For fuel injectors that dispense fine droplets of fuel in turbines, undesirable large droplets form during start-up and shut down in the 1 to 100 millisecond time frame. The ability to adjust the size and distribution of droplets on-demand based on a desired droplet size range could provide advantages in operation of jet engines to avoid flameouts. For example, jet engines that are operating at low power and low air flow or at high altitudes, where the density of air is low, benefit from small fuel droplets to improve control of combustion.

Inability to control the atomization process for atomization of molten metals

Limited ability of spray systems to provide high-precision, in-situ evaporative
to achieve a desired particle size distribution and achieve higher yield

For atomization of molten metal, there is a lack of understanding and technology to control \( d_{50} \) and produce a narrower powder size distribution with standard deviations close to 1. Lack of control of atomization hinders powder producers’ ability to produce a narrow particle size distribution and achieve higher yields. Ideally the ability to optimize narrow cut yields of powders with a 4:1 maximum-to-minimum size range is desired to meet customer specifications. Powder producers also want technology to minimize or eliminate the presence of satellite particles.

Lack of reliable, affordable refractory or ceramic materials that are resistant to reactive melts, especially to molten titanium

Due to the reactivity of molten metals, most metals are typically melted in furnaces or crucibles that are lined with refractory materials. In addition, ceramics or inert refractory materials such as boron nitride are typically used in atomizer nozzles. Because of the reactivity of titanium, “skull melting” is used to enable titanium to be melted in a water-cooled container lined with a frozen layer of titanium to avoid any contact with ceramic surfaces. Molten metal is also transported through ceramic tubes to the atomizing nozzle. Due to the limited selection of long-life and low-cost materials suitable for atomizer nozzles, there is a need for improved refractories and ceramics for atomization and melting.

Lack of a facility to test and evaluate new materials for atomization

Due to limited interaction among refractory material producers, manufacturers of melting furnaces, and commercial refractory part suppliers, there is a lack of knowledge of powder producer needs for longer life refractories. An atomizing facility that would be available for testing new and improved refractory materials will benefit supply chain vendors and companies that use refractory materials in critical atomizer components that are exposed to molten metals.

Lack of powder safety standards for titanium, aluminum, and magnesium production

Although safety guidelines for handling fine atomized powders have been issued by trade associations such as the Aluminum Association (The Aluminum Association TR-2), there is a need to promote awareness of current powder safety guidelines and to develop and adopt new guidelines. For example, additive manufacturing uses fine atomized powders, some of which are explosive. Methods to passivate powders for use in additive manufacturing to reduce the hazards associated with using powders in close proximity the laser or electron beam are also underdeveloped.

Priority R&D Activities

The challenges to improved process control of spraying of fuels, atomization of powders and thermal spraying processes can be addressed by the R&D activities listed in Figure 13. Priority activities are listed in bold and described in detail below.

Develop intelligent spray systems that are adaptive, on-demand, positive targeting, and based on feedback from real-time sensors and predictive models
### P7. Process Control

<table>
<thead>
<tr>
<th>Activity</th>
<th>Near (0–2 yrs)</th>
<th>Mid (3–4 yrs)</th>
<th>Long (5–10 yrs)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Develop intelligent spray systems that are adaptive, on-demand, positive targeting, and based on real-time sensing and predictive models</td>
<td></td>
<td></td>
<td>●</td>
</tr>
<tr>
<td>Establish development programs with refractory and ceramic part vendors to improve durability, precision, and performance of materials and parts (e.g., nozzles, stopper rods, tundishes)</td>
<td>●</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Develop a database of refractory material phase diagrams for specific melts</td>
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</tr>
<tr>
<td>Establish a safety/hazardous powders handling user’s group; update powder safety standards and create a database on explosibility of metal powders</td>
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<tr>
<td>Conduct workshops to discuss the needs of atomized powder producers with suppliers of equipment, process components, instruments and sensors.</td>
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<tr>
<td>Convene workshops with other industries that deal with molten metal or powders to seek best practice and technology transfer opportunities (e.g., casting, pharma, etc.)</td>
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<tr>
<td>Establish a common platform/language for atomization equipment</td>
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<tr>
<td>Develop methods to better control surface leveling and pore filling during spray deposition processes to eliminate trapped pores and reduce residual stresses</td>
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<tr>
<td>Understand the effects of process variations and instability on atomized powder quality</td>
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<tr>
<td>Investigate techniques for gas additions to improve powder passivation and reduce satellite powders</td>
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<tr>
<td>Investigate refractory and molten metal interactions for composite material systems (e.g., Ti, Ni)</td>
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<tr>
<td>Develop new spray deposition techniques with powders of different materials through the same nozzle</td>
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<td></td>
<td></td>
</tr>
<tr>
<td>Define a strategy to develop more efficient cost-effective, pre-competitive new atomizing methods</td>
<td>●</td>
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<tr>
<td>Enable control of particle/droplet size distribution (e.g. d50, d90, and d10) and particle shape, and eliminate attached satellite powders as a function of process parameters and atomizer set-up</td>
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<td></td>
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<tr>
<td>Conduct collaborative studies on step-change (disruptive) process control technologies to adjust particle size and increase yield</td>
<td>●</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Obtain funding for research on improved ceramics for processing molten metals that are ITAR restricted</td>
<td>●</td>
<td></td>
<td></td>
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<tr>
<td>Perform research to identify and quantify effects of parameters on water/gas atomization</td>
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</table>
There is a strong desire to develop rapidly adjustable spray control actuators for nozzles, especially for use in harsh environments such as jet turbine engines, to enable active droplet size control of the droplet size or spray pattern during operation. Development of intelligent spray systems will require comprehensive and integrated efforts to design injectors that can respond to changes in the fluid flow. Development of real-time sensors and algorithm models for analysis of sensor data is needed for active control of sprays by using rapidly adjustable spray control actuators to allow active in-situ droplet size or spray pattern control. Consideration may be given to evaluating variable geometry nozzles (e.g., nozzles with an adjustable orifice) to achieve the desired droplet size.

Establish development programs with refractory and ceramic part vendors to improve durability, precision, and performance of materials and parts (e.g., nozzles, stopper rods, tundishes)

Investigation of better refractory materials and best practices for improved refractory performance are required to extend the life of refractory components and reduce the probability of contamination of powders.

Develop a database of refractory phase diagrams for specific melts

Reviewing current phase diagrams and establishing a database of refractory materials for use with specific molten metal alloys can improve materials selection and reduce the probability of contamination of molten alloys. Refractories that can contain molten titanium alloys pose especially significant challenges.

Establish a safety/hazardous powders handling user’s group; update powder safety standards and create a database on explosibility of metal powders

A number activities can be undertaken to improve safety of handling metal powders. Initially a team from industry can collect “best practice” powder safety guidelines that are based on industrial practices. The team should also collect information from the National Fire Protection Association (NFPA), MPIF, SAE, Aluminum Association or other organizations to obtain information on powder safety and standards such as NFPA 652. The team should review and summarize the current powder safety standards and explosibility testing procedures (e.g., ASTM Standard E1226), and create a database on explosibility of metal powders. Investigation of techniques to improve powder passivation by gas additions would facilitate safer handling of powders for reactive alloys. Passivation may also reduce the amount of satellite powders that attach to powders as the powders are transported to the collection system. In addition to updated standards on powder safety, workforce training of existing and new personnel that atomize and handle fine powders is needed for improved safety.

Develop methods to better control surface leveling and pore filling during spray deposition processes to eliminate trapped pores and reduce residual stresses

For thermal sprayed deposits, develop new spray deposition techniques with powders of different materials through the same nozzle to produce uniform dense coatings with low levels of residual stress.
Understand the effects of process variations and instability on atomized powder quality

Maintaining the size, distribution, and shape of atomized molten metal droplets that rapidly solidify to form powders requires an understanding of how changes in process parameters can affect powder characteristics. During steady-state atomization, variations in molten metal temperature, changes in atomizing gas or water temperatures, fluctuations in gas or water pressures, and changes in the size of the nozzle inside diameter due to erosion can alter the powder size and distribution. A systematic study of the effect of variations in key process parameters needs to be conducted so methods to control process variables can be developed.

Enable control of particle size distribution (e.g., d50, d90, and d10) and particle shape, and eliminate attached satellite powders as a function of process parameters and atomizer set-up

Establishing the capability to atomize powders within defined powder size ranges, without satellite attached powders, will enable powder producers to consistently meet customer specifications. To achieve this goal, an improved level of process understanding is needed. In some cases, process models with input from real-time imaging and in-situ sensors can be used by actuators to control the flow of gas, air, or water or to adjust other process parameters.
PATH FORWARD

The use of atomization and spraying technologies in such a wide range of manufacturing applications means that even modest improvements in powder characteristics and spray performance can provide substantial benefits. Widespread increases in efficiency and productivity can help to support a growing and more competitive U.S. manufacturing sector. The R&D activities identified in this roadmap chart the course for future technology advances that, if realized, can accelerate this potential outcome.

To ensure that the coordinated efforts to develop and implement advanced atomization and spray technologies continue to build momentum, ASM International is working with leaders in atomization and spraying to establish the Atomization Technology Innovation Consortium (ATIC). The goal of ATIC is to serve as an organizing body for cross-industry atomization and spraying technology communities and provide a forum for industry and academia to share pre-competitive knowledge and work together to develop solutions that can be implemented by industry. ATIC can also function as an interface with non-member companies to help protect intellectual property of member companies and to ensure adequate vetting of potential supply chain vendors, especially non-domestic vendors. By connecting the right people and cultivating a collaborative environment, ATIC will help tap into the nation’s leading expertise to increase control of atomization and spray processes and revolutionize the ways they can be used to drive growth in U.S. manufacturing.

Figure 14. ATIC: An enabler of collaboration among atomization and spraying communities
APPENDIX A. APPLICATIONS OF ATOMIZATION AND SPRAYING TECHNOLOGIES

As shown in Table A1, two-fluid and single-fluid atomization and spray processes are used in a wide variety of industries to produce particles or droplet sizes to meet the requirements of specific applications. For example, two-fluid or single liquid hydraulic nozzles are used in a wide variety of industries and applications including chemical production, paper manufacturing, painting, and cooling. For the production of powders, gas or water atomization is extensively used; however specialized single-fluid atomization processes such as centrifugal, ultrasonic, spray drying, and other methods are used to produce powders or granules for specific applications. Jet turbines, land-based turbines, and internal combustion engines rely on specially designed injector nozzles to produce sprays of fuel droplets combustion.

Table A1. Atomization and Spraying Processes, Industries, and Applications

<table>
<thead>
<tr>
<th>Industry: Application</th>
<th>Two-Fluid Processes</th>
<th>Single-Fluid Processes</th>
</tr>
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<tbody>
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<td>Atomization Methods</td>
<td>Special Atomized Sprays</td>
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<td>Water or Oil / molten metal</td>
<td>Gas: (Air, N₂, Ar, He) / molten metal</td>
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<td>Two-Fluid Processes</td>
<td>Single-Fluid Processes</td>
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<td>Atomization Methods</td>
<td>Special Atomized Sprays</td>
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<td>Paper manufacturing</td>
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<tr>
<td>Paints, adhesives, lubricants</td>
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<tr>
<td>Coatings</td>
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<td>Cooling rolls</td>
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<tr>
<td>Fire suppression</td>
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<tr>
<td>Ink jet</td>
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<tr>
<td>Consumer products/food</td>
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<td>Powder Metallurgy</td>
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<td>Powder metal production</td>
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<td>Metal injection molding</td>
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<td>Additive manufacturing</td>
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<td>Spray forming</td>
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<td>Internal combustion engines</td>
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<tr>
<td>Rocket engines</td>
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</table>
APPENDIX B. ROADMAP CONTRIBUTORS

The following individuals made valuable contributions to this roadmap by participating in roadmapping workshops, expert interviews, and serving on the ATIC Leadership Team.

**Chris Adam**  
Royal Metal Powders, Inc.

**James Adams***  
Metal Powder Industries Federation

**Guillermo Aguilar**  
University of California-Riverside

**Nasser Ahmad**  
North American Höganäs, Inc.

**Iver Anderson***  
Ames Laboratory

**Ross Brindle**  
Nexight Group

**Daniel Bissell**  
TSI Incorporated

**Kyle Blakely**  
Eli Lilly and Company

**Jung-Hoon Chun**  
Massachusetts Institute of Technology

**Bidhan Dam**  
Woodward Inc.

**Olivier Desjardins**  
Cornell University

**John Dunkley**  
Atomizing Systems Limited

**Rob Gorham***  
America Makes

**Mark Hash**  
Ervin Industries Inc.

**Greg Hildeman**  
Nexight Group

**Andrew Heidloff**  
Praxair Surface Technologies

**Scott Henry***  
ASM International

**Marcus Herrmann**  
Arizona State University

**Greg Hildeman**  
Nexight Group

**Jessu Joys**  
United States Metal Powders, Inc.

**Malissa Lightfoot**  
Air Force Research Laboratory, Edwards Air Force Base

**Deepak Madan**  
Magnesium Elektron Powders

**Bernard Mais**  
ECKA Granules

**Adel Mansour**  
Parker Hannifin Aerospace

**Vincent McDonell***  
University of California-Irvine Combustion Laboratory

**Bailie McNally**  
Worcester Polytechnic Institute

**John Meyer**  
Carpenter Technology Corporation

**Robert Miller***  
R.A. Miller Materials Engineering

**Dave Milligan**  
North American Höganäs, Inc.

**Bill Mosier**  
Polymet Corporation

**Todd Palmer***  
Pennsylvania State University

**Scott Parrish***  
General Motors Research and Development

**James Perozzi**  
AMETEK

**Stamatios Pothos**  
TSI Incorporated

**Chris Powell**  
Argonne National Laboratory

**Jim Sager**  
Woodward Inc.

**Chris Schade**  
Hoeganaes Corporation

**Jim Sager**  
Woodward Inc.

* Member of the ATIC Leadership Team
**APPENDIX C. ACRONYMS AND ABBREVIATIONS**

<table>
<thead>
<tr>
<th>Acronym</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>d50</td>
<td>median mass diameter where 50% of the liquid droplet or powder mass is above and below the given size</td>
</tr>
<tr>
<td>d10 or d90</td>
<td>mass diameter where 10% or 90% respectively of the liquid droplet or powder mass is below the given size</td>
</tr>
<tr>
<td>AM</td>
<td>additive manufacturing</td>
</tr>
<tr>
<td>CFD</td>
<td>computational fluid dynamics</td>
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<td>DNS</td>
<td>direct numerical simulation</td>
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<td>HPC</td>
<td>high-performance computing</td>
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<td>LES</td>
<td>large eddy simulation</td>
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<td>MIM</td>
<td>metal injection molding</td>
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<td>PM</td>
<td>powder metallurgy</td>
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<tr>
<td>PDA</td>
<td>phase Doppler anemometry</td>
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<tr>
<td>PDPA</td>
<td>phase Doppler particle analysis/analzyer</td>
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<td>PIV</td>
<td>particle image velocimetry</td>
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<tr>
<td>PSD</td>
<td>particle size distribution</td>
</tr>
<tr>
<td>SMD</td>
<td>Sauter mean diameter</td>
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</table>
APPENDIX D. REFERENCES


U.S. Census Bureau. 2014. “Annual Survey of Manufacturers (ASM).”


