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DIGITAL TWIN AND FLOW SIMULATION FOR IMPROVED MATERIALS PROCESSING

Beyond simulation, the real power of a digital twin is the closed feedback loop, which provides valuable digital-side visualization, enabling accelerated materials development.

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A digital twin is a system that copies a real object—a product, a piece of equipment, a process—into a digital space. This digital copy is updated with data from the real world and uses the results of the analysis to improve the real object.

Closing this loop—visualizing behavior in a digital space, feeding the results back into the real world for testing, and sending the verified data back to the digital side again—can move research and development forward a great deal, in either field. The closed loop is the gate through which digital twins will open a new frontier for materials science. This article introduces one such attempt at digital-side visualization, built on a particular software platform.

As described in the box below, the

authors' research interests are centered around additively manufactured metal powders and bacteria-based biofilms. In both fields, the usual approach is trial and error, repeating the experiment and adjusting it in search of a good solution. This is slow, it costs money, and it is reaching its limits.

A DIFFERENT KIND OF SOLVER: PARTICLES, NOT MESHES

Most computer-aided engineering (CAE) tools for fluid and particle flow are built on a mesh: The domain is divided into a fixed grid of elements or cells, and the equations are solved on that grid. Finite element and finite volume methods have done this job well for decades. But a fixed mesh has trouble when the shape of the domain itself keeps changing—a free surface

sloshing, particles separating and coming back together, a powder bed collapsing under a blade. Each time the free surface or the particle arrangement moves far enough, the mesh has to be rebuilt to keep up. This costs computing time and can also be a source of numerical error.

This study utilizes two platforms from Prometech Software—Particleworks and Granuleworks. Each takes a different approach. Both are particle methods: The fluid or the granular material is represented directly as a set of particles that interact with each other, not as values fixed to a grid. Thus, there is no mesh to distort or rebuild as the powder moves. Particleworks was developed first as a general fluid solver for problems such as gearbox lubrication. Granuleworks extends the

AUTHORS' RESEARCH FOCUS

Two of the article's authors, Dr. Jeremy Knopp and Dr. Takayoshi Nakano, work on laser-based additive manufacturing of metal powders. The other two authors, Dr. Hideyuki Kanematsu, FASM, and Akiko Ogawa, work on accelerated-test devices for the laboratory evaluation of biofilms formed by bacteria on material surfaces.

In 2025, they presented the biofilm case in part at the International Materials, Applications, & Technologies (IMAT) conference in Detroit, and the powder case for additive manufacturing (AM) technology at the Materials Science & Technology (MS&T) 2025 event. As the latter meeting was held in Ohio, the authors also delivered an invited lecture at Wright State University in Dayton. They hope to report on the physical-space results at an IMAT conference in the near future.

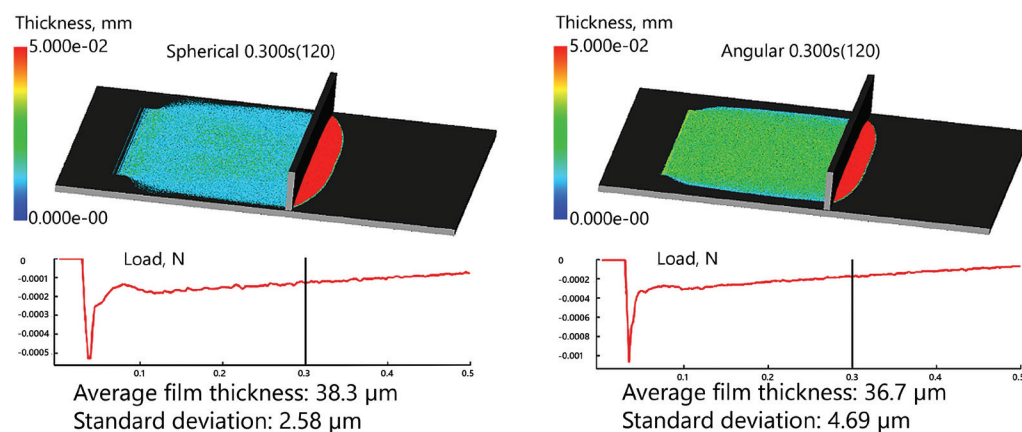


Fig. 1 — Effect of particle shape on powder spreading with a blade-type recoater: spherical particles (left) vs. angular particles (right). It was found that particle friction causes nonuniformity in film thickness. Created with Prometech Software.

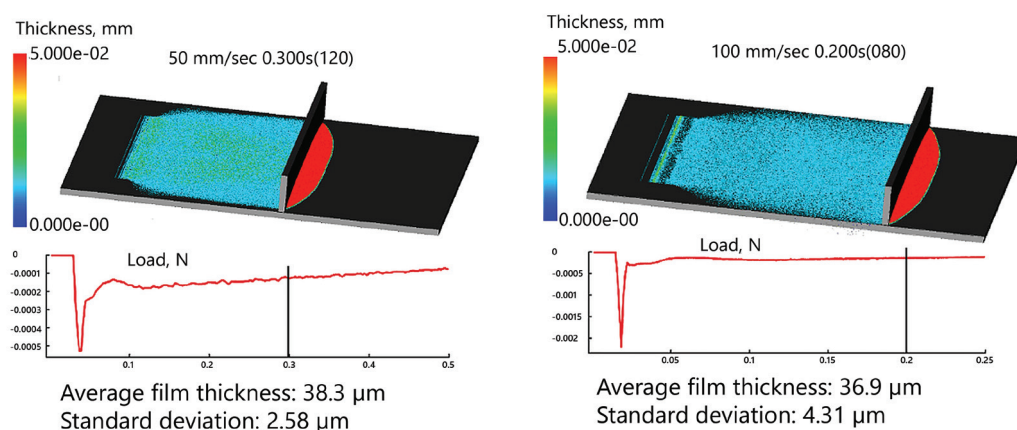


Fig. 2 — Effect of blade speed on powder spreading with a blade-type recoater: 50 mm/s (left) vs. 100 mm/s (right). It was found that overall film thickness decreases as the blade speed increases. Created with Prometech Software.

same particle idea to granular solids—gravel, sand, snow, and, in this case, metal and ceramic powders. The two platforms couple directly, allowing the operator to follow one powder through the free-flowing stage of a hopper discharge and the dense, packed stage of a spread layer, all in one simulation, instead of connecting separate solvers.

APPLICATION EXAMPLE 1: POWDER BED FUSION

The first example began with a basic check: comparing powders of high and low surface energy as they flowed from a hopper. The result was clear. The low surface-energy powder flowed at 13.9 g/s, and the high surface-energy powder flowed at only 11.0 g/s—about a 20% drop. Higher surface energy means stronger cohesion

between particles and less free flow in a powder bed. This is the same result observed in the biofilm example below, where higher surface energy also means stronger initial bacterial attachment on a coupon.

The team then moved to a geometry closer to the real process: powder spreading with a blade-type recoater, the part used in most powder-bed-fusion AM systems to lay down each layer. Here the surface-energy effect showed up not only in speed but in uniformity. The low surface-energy powder gave an average spread-film thickness of 38.3 μm, with a standard deviation of 2.58 μm—tight and consistent. The high surface-energy powder gave a slightly thinner average of 36.4 μm, but the standard deviation was 4.62 μm, almost double the scatter. Thus, the more cohesive powder does

not only move more slowly, it also spreads less evenly. This kind of layer-to-layer variation is what later shows up as porosity or dimensional error in the finished part.

Particle shape had a similar effect. Spreading spherical particles with the same blade-type recoater gave an average film thickness of 38.3 μm, with a standard deviation of 2.58 μm. Angular particles gave a close average, 36.7 μm, but the standard deviation rose to 4.69 μm (Fig. 1). The extra scatter comes from friction: Angular particles catch on each other as they move, and that friction is what makes the layer less even, not a change in the average amount of powder laid down.

Blade speed mattered too. At 50 mm/s, the recoater produced the same 38.3 ± 2.58 μm layer. At 100 mm/s, the average thickness dropped a little, to 36.9 μm, and the standard deviation rose to 4.31 μm (Fig. 2). A faster blade does not just move the powder faster—it also leaves a slightly thinner, less even layer. Unlike particle shape or surface energy, which are set by the feedstock, blade speed is a parameter a manufacturer can adjust directly on the machine.

APPLICATION EXAMPLE 2: DESIGNING A FLOW-BASED BIOFILM REACTOR

Biofilms form on material surfaces without exception, so in a sense, a biofilm is a kind of material-surface degradation. But historically, materials scientists and engineers have not looked at this problem enough from their own point of view, and this could be one important reason why research and development in this area, and the

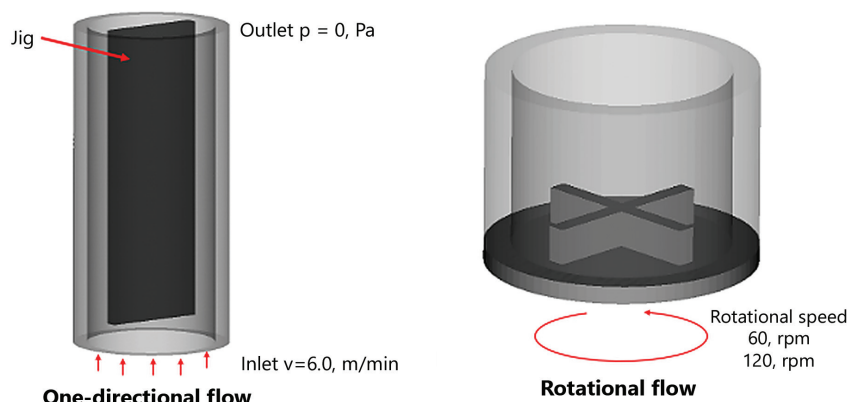


Fig. 3 — Simulation model for the two candidate biofilm reactors: (left) a vertical column-type reactor with one-directional flow (inlet velocity 6.0 m/min) and (right) a horizontal stirred-tank reactor with rotational flow (60/120 rpm). Created with Prometech Software.

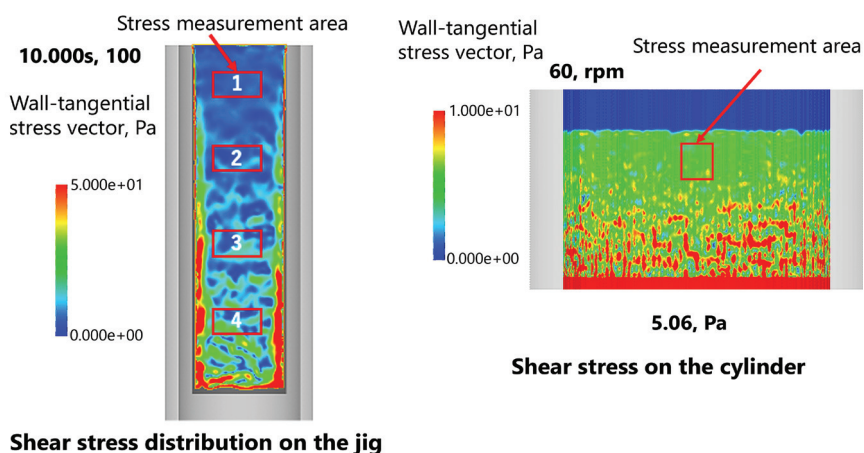


Fig. 4 — Simulated wall shear stress: distribution on the jig in the column-type reactor (left) and on the cylinder wall in the stirred-tank reactor (right). Created with Prometech Software.

practical problems it should solve, have lagged behind. To address this concern, the authors have proposed several biofilm test methods. Among the variables these methods need to control, flow turned out to be an especially important one, and a laboratory-scale reactor that brings flow under control has been needed for some time.

Two reactor designs are proposed based on this idea (Fig. 3). The first is a vertical column-type reactor, working as a plug-flow reactor, where a test coupon sits in a one-directional, upward flow. The authors have already built and used this design in the lab. But a column-type reactor can only hold a limited number of coupons at once, so running enough trials for solid conclusions takes a lot of time. The second design is meant to solve this problem: a horizontal, stirred-tank

reactor, where a rotating impeller drives a circulating flow around coupons placed in the tank, instead of the one-directional flow of the column. The aim is for this stirred-tank design to give the same biofilm-forming ability as the column-type reactor, while allowing for many more coupons to be tested at the same time.

The authors believe shear stress at the material surface is the variable that controls how easily a biofilm forms. So before building the physical design, they used particle-based simulation to calculate the wall shear stress for both reactor shapes (Fig. 4). In the column-type reactor, shear stress on the coupon surface increased toward the lower part of the flow path, because the flow becomes more turbulent there. In the stirred-tank reactor, shear stress was concentrated near the wall

and increased with impeller speed—from about 5.1 Pa at 60 rpm to about 5.7 Pa at 120 rpm on the cylinder wall. From these results, an impeller speed and coupon placement can be chosen that give, in the stirred-tank reactor, a shear-stress environment close to the one already confirmed in the column-type reactor. The working idea is that matching the shear environment should also give comparable biofilm-forming behavior, and the next step is to check this directly against coupon data from both reactors.

FOR THE FUTURE

These two examples show how visualization on the digital side can be fed back into the real world. This is different from a simple simulation. The aim is a closed loop: feedback experiments in the real space, then feedback again to the virtual side, and a new round of study starting there. This closed loop is what a true digital twin means, and we are working on it now. This digital-twin approach makes it possible to repeat experiments in a way that was not possible before, and to reach the right answer in physical space through this new experimental style. As virtual space and artificial intelligence continue to develop, the authors have a strong feeling that this will become the standard way of doing things. ~AM&P

Acknowledgments

The authors thank Prometech Software Inc. for kindly providing the simulation images used in Figs. 1-4 of this article. They also are grateful to PacForce K.K. for arranging this collaboration.

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