The 55th William Blum Lecture
Presented at NASF SUR/FIN 2021
in Detroit, Michigan
November 2, 2021

Modeling and Simulation for the Finishing Industry

by
Dr. Keith Legg
Recipient of the 2019 William Blum
NASF Scientific Achievement Award

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Editor's Note: The following is based on the Powerpoint presentation by Dr. Legg in delivering his William Blum Memorial Lecture at SUR/FIN 2021, in Detroit, Michigan on November 2, 2021. Dr. Legg was announced as the recipient of the 2019 NASF William Blum Scientific Achievement Award at SUR/FIN 2019 in Chicago (Rosemont), Illinois.

EXTENDED ABSTRACT[*]

As Dr. Legg watched the changes in industry over the past decade or so, he has seen modeling and simulation move from one industry to another. Seeing how and where it is used elsewhere, he concludes that modeling could be more widely and profitably used in the surface finishing industry.

Models are not reality, but they are tools to make reality more comprehensible and predictable. Models give us a way to predict the behavior of complex systems, find ways to improve their performance, and change the outcome. In evolving from trial and error design to computational design, outcomes in fluid dynamics, stress, heat transfer and corrosion modeling can be rapidly predicted.

If only the Wright brothers had had access to computation fluid dynamics. More modern examples include the fluid dynamic in appliances, such as dishwashers. Fluid dynamics determines the forces on aircraft and cars and its study is used to visualize fluid flow, measure lift, drag forces, etc. We used to employ wind tunnels, which are very expensive and yield limited quantitative data. With computational fluid dynamics (CFD) modeling, the computer to do this fits in the trunk of a car and a great deal more data is gathered. Advanced materials characterization techniques can be used to advance materials design. Numerous thermodynamic and materials modeling methods have been used to develop new alloys in weeks rather than years. CFD can be used to determine the flow of gases or droplets in a room, allowing better ventilation.

However, a model is only as good as what goes into it. A model must include all the critical processes and have good quality data. This does not mean it must be all-encompassing to be useful, but one needs to know what its limitations are, where it is valid and where it will break down. For example, if your product contains dissimilar materials, a galvanic corrosion model may be fine, but if you have a lot of overlapping components, you probably need a crevice corrosion model as well. If your product is used on a ship, you need seawater corrosion data, but if it is used in a chemical plant, you may need acid corrosion data.

How does one know that a model is any good and whether it is useful? It may look nice but is the model validated against good data? Does it hindcast? That is, does it predict known data – qualitatively, quantitatively? If the validation data is not accurate, it is missing something important. The complexity of the system to be modeled is critical. The more complex it is, the harder it is to be sure it includes all the critical variables. One also needs to know how accurate it must be to get useful answers and what are the consequences of a wrong answer?

The most important thing that modeling is that it gives you the insight to improve processes and handle change efficiently, with a

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[*] Compiled by Dr. James H. Lindsay, NASF Technical Editor.

lot more certainty. It is almost always far faster and cheaper to develop and optimize materials and processes using modeling than using formulation and testing. This is particularly important for developing and optimizing coatings.
When your product or process has to change, you may need to redesign a component. A model lets you quickly check how you will affect system performance. If regulations such as REACH bans yet another of your critical chemicals or coatings, you must first get the materials data from the alternatives. Then, you can quickly rerun your models with all the alternatives to see how performance changes (Cr6 > Cr3 > non-Cr). if you want to enter a new market, you can model performance directly over the entire product for all manner of stresses and environments. You can reduce risk by evaluating any number of what-ifs – far more than you could possibly test. This includes checking for possible but unusual scenarios that would not happen in normal service testing – or that would be disastrous if they did.

For example, in automotive component plating, both Ford and GM both encourage or require computational modeling to ensure coating thickness uniformity on plating-on-plastic parts. Some companies always carry out computational modeling whether the customer requires it or not, (1) to meet specifications for thickness uniformity across components and across the plating rack and (2) to optimize the loading on the rack for maximum throughput consistent with coating quality. Some companies that design, mold and plate also use CFD to optimize mold filling, ensure part quality, platability and plating quality.

So, why use modeling in surface finishing and corrosion? While stress engineers, heat transfer engineers and vibration engineers all have models showing why their solutions will work, the corrosion/coatings engineer cannot prove (even to himself) that his solution will work. Without quantitative modeling, the corrosion/coatings is severely handicapped.

Models don't have to be complicated to be useful, but they do have to be correct. Getting it right means you must define the way the model is made, where it is valid, and how to take the data that go into it.

In the corrosion modeling standard MIL-STD-889D, NAVAIR improved the original *Best Practices for Data Acquisition - Polarization Data for Galvanic Corrosion Protection* and incorporated them into MIL-STD-8809D. Naval aircraft operate off aircraft carriers – the world's most corrosive environment. One concern involved the corrosion protection of bushings and fasteners where an aluminum-rich primer needed to be evaluated as a cadmium plating replacement. Proper evaluation required hundreds of formulations, thousands of tests, and millions of dollars. With modeling, it did take a couple of years to develop the model and measure the underlying electrochemical properties of its constituents, but once model was developed, CFD workflow automation took days instead of weeks. Optimization took thousands of simulations over a few weeks, and the optimum formulation was defined.

Another example involves the replacement of Cd in aerospace and Zn in automotive with ZnNi plating. It is easy to plate an element - get the plating parameters right and Faraday's law takes care of the rest. Once you have two elements however, they don't necessarily deposit in the same ratio as the composition in the electrolyte, and that ratio can vary with plating voltage, current density, electrolyte flow rate, etc., meaning that the coating chemistry, microstructure and performance can vary across complex components. You can even go from galvanically protective to galvanically corrosive in different areas. If you want to plate ZnNi for aerospace, your tooling must be designed by electrodynamic simulation and sometimes computational fluid dynamics to get the right chemical and thickness uniformity. The Zn/Ni ratio varies with current density and current density varies over complex shapes, holes, etc., so one must model component, anodes, secondary anodes and robbers. Complex parts may also require modeling fluid flow modeling, using eductors.

Machining turbine engine components, gun rifling and other complex parts, often involves electrochemical machining (ECM). However, the ECM tool rapidly corrodes holes in very hard alloys. Hole dimensions, however, are a complex function of tool shape, voltage, etc. • The only way to design a tool is multiple iterations of trial and error, which is very costly and uncertain. It takes many months and even then, you may not get good enough tolerance. A possible solution is to develop an ECM model to calculate the required tool shape, provided you model a process with so many variables: electrochemical properties of the tool, workpiece alloys, and the electrolyte, the use of DC or pulsed current, the machining rate and removal of heat, debris, bubbles, etc. Ideally, we should be able to mathematically unmachine the part to determine the tool from the finished product. However, it turns out we cannot do that, but we can model hundreds of tool shape iterations to optimize the tool. Once the ECM model exists, we can quickly and reliably design tools to machine any shape.

Another example involves non-drip brush plating. For the tool to be non-drip, the fluid moving out of the pad must be balanced by the air flowing in. Whenever we design a new non-drip brush plating system, we use a combination of computational fluid dynamics and electrodynamics to ensure the tool will not drip and will plate uniformly. With computational methods, a non-drip repair system to repair Al anodizing and fastener corrosion on an aircraft wing simultaneously was developed. On-aircraft processing at this scale could be done without computational methods.

Today, modeling for surface finishing is a recognized approach. It is proving to be very useful for plating and some finishing processes. It is finding new uses as it develops, but there is a lot to learn. The aim is to make modeling a standard, integrated approach to coating development and corrosion protection.

About the author

Dr. Keith Legg, is Co-owner and CTO of Corrdesa LLC, Newnan, Georgia, a new venture started by Alan Rose and Keith Legg to bring computational galvanic corrosion prediction software to the market for design and maintenance. Corrdesa works closely with various defense organizations and aerospace companies to use the computational approach for assessing risk and correcting design.

He is also President of Rowan Technology Group, Chicago, Illinois, a consulting organization specializing in coatings and surface treatments. He is also Technical Manager of the ASETSDefense DoD Initiative, which provides information, a public database of reports, periodic workshops and assistance to engineers to meet ESOH requirements for US and Europe.

Dr. Legg earned his B.A. in Physics from Lancaster University (UK)(1967-1970) and his D. Phil, in Physics from the University of York (UK)(1970-73). His expertise is in advanced coatings and alternatives to materials and coatings with environmental and health problems, such as chromate materials and processes, chrome plating, Cd plating, etc.