



Summary: ASETSDefense 2011

Side meeting on Computational and Database Methods

The briefings are now posted on the ASETSDefense website at:
<http://www.asetdefense.org/SustainableSurfaceEngineering2011.aspx>

Date: February 7, 2011

Author: Keith O. Legg

ASETSDefense Technical Manager

Contact information:

Dr. Keith O. Legg

Rowan Technology Group, 1590 South Milwaukee Ave, Suite 205, Libertyville, IL 60048

Tel: 847-680-9420, Fax: 847-680-9682

Email: klegg@rowantechnology.com

TABLE OF CONTENTS

1. Agenda.....	- 1 -
2. Briefings	- 1 -
2.1. Introduction (Keith Legg)	- 1 -
2.2. DoD Needs and Vision (Craig Matzdorf, NAVAIR).....	- 2 -
2.2.1. Design Modules for Corrosion Protection (Farrell Martin, ONR).....	- 2 -
2.2.2. Durable Aircraft (Craig Matzdorf, NAVAIR)	- 3 -
2.3. Computational Galvanic Corrosion Protection (Leslie Bortels and Alan Rose, Elsyca).....	- 4 -
2.4. Coatings Databases (Patrick Coulter and Will Martin, Granta Design).....	- 4 -
2.5. Galvanic Data Acquisition (Dennis Dull, Boeing).....	- 5 -
2.6. cWorks (Steve Gaydos, Boeing)	- 6 -
2.7. Corrosion Prevention and Control Database (Bob Barbin, Matt Koch, USMC CPAC)	- 7 -
2.8. Materials by Design (Charles Kuehmann, Questek Innovations)	- 8 -
2.9. Atoms to Airplanes, the Future (Joe Osborne, Boeing).....	- 9 -
3. Summary.....	- 9 -

LIST OF FIGURES

Figure 1. Overview of relationships between databases, computational methods and system performance....	- 2 -
Figure 2. ONR database, modeling and prediction approach (Farrell Martin).	- 3 -
Figure 3. Corrosion test and design hierarchy. (Craig Matzdorf).....	- 3 -
Figure 4. Galvanic Master galvanic corrosion prediction software (Elsyca).	- 4 -
Figure 5. Vision of the Coatings Database and its fit with predictive software (Granta).	- 5 -
Figure 6. Next-generation galvanic series (Dennis Dull).	- 6 -
Figure 7. cWorks output for design (Steve Gaydos).....	- 7 -
Figure 8. Data structure of the USMC CPAC database (Bob Barbin).	- 8 -
Figure 9. Materials by design compared with traditional empirical alloy development (Questek).....	- 8 -
Figure 10. Wind shear acting on what control what on smooth and rough surfaces (Joe Osborne).	- 9 -

1. Agenda

Monday, February 7, 2011		
Side Meeting: Computational & Database Methods for Design & Prediction		
1300	Introduction	Keith Legg ASETSDefense
1310	Durable Aircraft, Design Modules for Corrosion Protection	Craig Matzdorf, Farrel Martin NAVAIR, NRL
1340	Computational Galvanic Corrosion Prediction	Leslie Bortels Elsyca (Belgium)
1410	Coating Databases for Aircraft & Weapon Systems Design, Incorporating Performance, Galvanic, Environmental & Cost Data	Patrick Coulter Granta Design (UK)
1440	Galvanic Data Acquisition	Dennis Dull Boeing Research & Technology
1455	Break	
1515	cWorks - Corrosion Identification and Management Software for Aircraft Corrosion Control	Steve Gaydos Boeing Research & Technology
1545	Corrosion Prevention and Control Database	Bob Barbin, Matt Koch USMC CPAC
1615	Materials by Design - Computational Alloy Design for Corrosion Control	Charlie Kuehmann Questek Innovations
1645	Atoms to Airplanes: The Future	Joe Osborne Boeing Research & Technology
1715	Discussion	
1800	Adjourn	

All of the briefings are available on the ASETSDefense website at

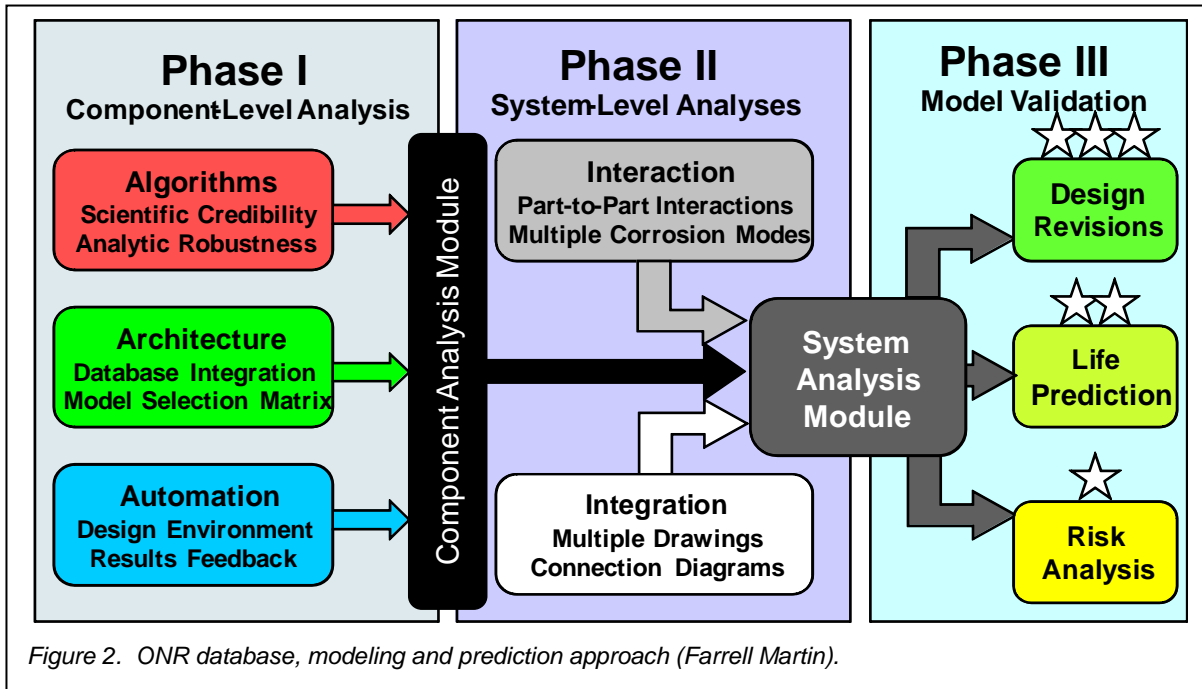
<http://www.asetdefense.org/PastWorkshops.aspx>

2. Briefings

2.1. Introduction (Keith Legg)

Keith Legg provided a brief overview of the genesis of the session and how the various databases and computational methods could link together (see Figure 1) to create a methodology for designing more reliable and higher performance weapons systems on a shorter time scale by linking all the way back to design of the materials themselves. Success will depend on reliable and consistent data held in databases capable of interacting with modeling software, which in turn must integrate into design software. Designs can then incorporate material and coating properties and performance, together with system experience, to avoid the mistakes that we have often seen, especially in areas such as galvanic corrosion.

We are still a long way from this integrated picture, but a number of its building blocks are now in place.



2.2.2. Durable Aircraft (Craig Matzdorf, NAVAIR)

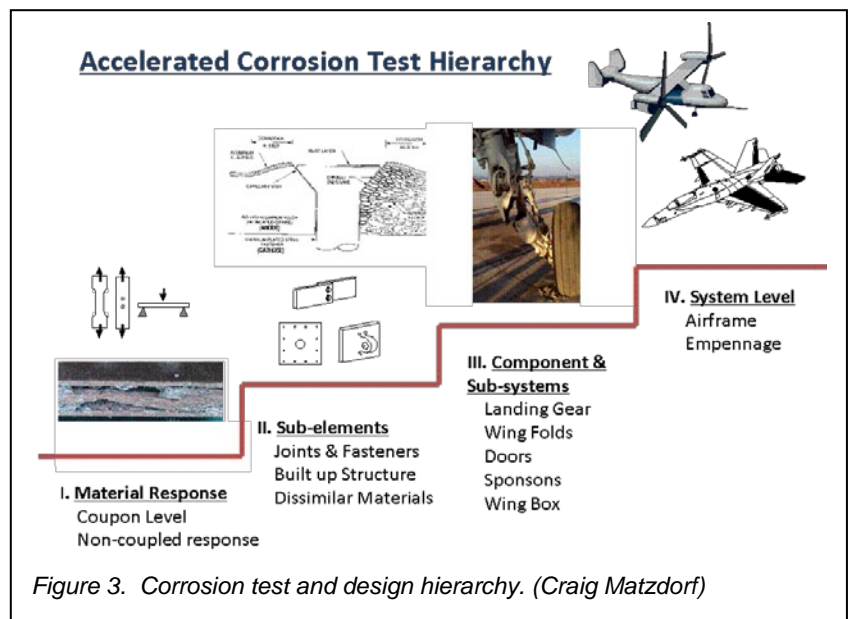
Craig provided an overview of NAVAIR's long-term vision for Durable Aircraft.

- Vision
 - Develop galvanic management technologies and engineered systems that eliminate fleet maintenance and reduce life-cycle corrosion costs of aircraft (see Figure 3).
- Major Focus Areas
 - Integrated Structural and Corrosion Design Tool
 - Tests for Prototyping Corrosion
 - Engineered Interfaces and Materials

Electric potential is the primary driver for corrosion in Naval air systems, with the main factors being

- EM Environment
- Weather / Op Environment
- Dissimilar Materials
- Stress
- Design
- Coatings
- Material Degradation

Thus the issue is not simply one of corrosion, nor purely galvanic corrosion, but includes the effect of impressed currents, the operational environment, and degradation of the coatings, including generation of corrosion products and loss of inhibitors. Technology solutions will focus on F/A-18, H-60, E-2, H-53 a/c and future platforms - N-UCAS, F/A-XX.



2.3. Computational Galvanic Corrosion Protection (Leslie Bortels and Alan Rose, Elsyca)

Leslie and Alan described and demonstrated Elsyca's commercial Galvanic Master approach to modeling and predicting galvanic corrosion in components and systems using multiple materials and complex shapes. This software is designed to work with CAD software, and to be usable by engineers with no experience in finite element analysis. It produces three-dimensional drawings showing corrosion rates over the entire surface (see Figure 4).

This system is based on the following principles:

- Physics-based – solves the fundamental electrochemical equations
- CAD-based – takes into account full geometrical configuration from the CAD drawings for the system
- Real-life based – using measured polarization curves as input (standard methodology), not just galvanic potentials
- Validated – by tier 1 automotive supplier and aerospace supplier on existing components
- Available – industrially deployed, user-friendly, fast solver, automatic reporting.

Group	Surface area [cm ²]	Average [um/year]	Minimum [um/year]	Maximum [um/year]	Deviation [um/year]
Al1	524.05	131.3	2.6	873.5	171.0
Al2	556.26	106.1	0.8	898.5	148.6
Copper1	22.28	0.00	0.00	0.00	0.00
Copper2	22.30	0.00	0.00	0.00	0.00
Copper3	22.27	0.00	0.00	0.00	0.00
Copper4	22.27	0.00	0.00	0.00	0.00
Copper5	22.27	0.00	0.00	0.00	0.00
Copper6	22.28	0.00	0.00	0.00	0.00
Steel1	22.57	0.00	0.00	0.00	0.00
Steel2	22.62	0.00	0.00	0.00	0.00
Steel3	22.62	0.00	0.00	0.00	0.00

Table 11: Corrosion rate/year (based on 40 days of rain/year)

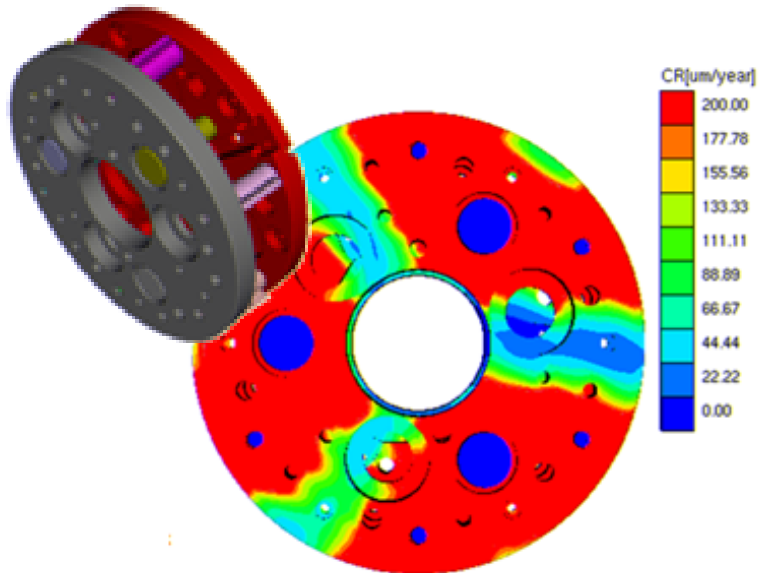


Figure 4. Galvanic Master galvanic corrosion prediction software (Elsyca).

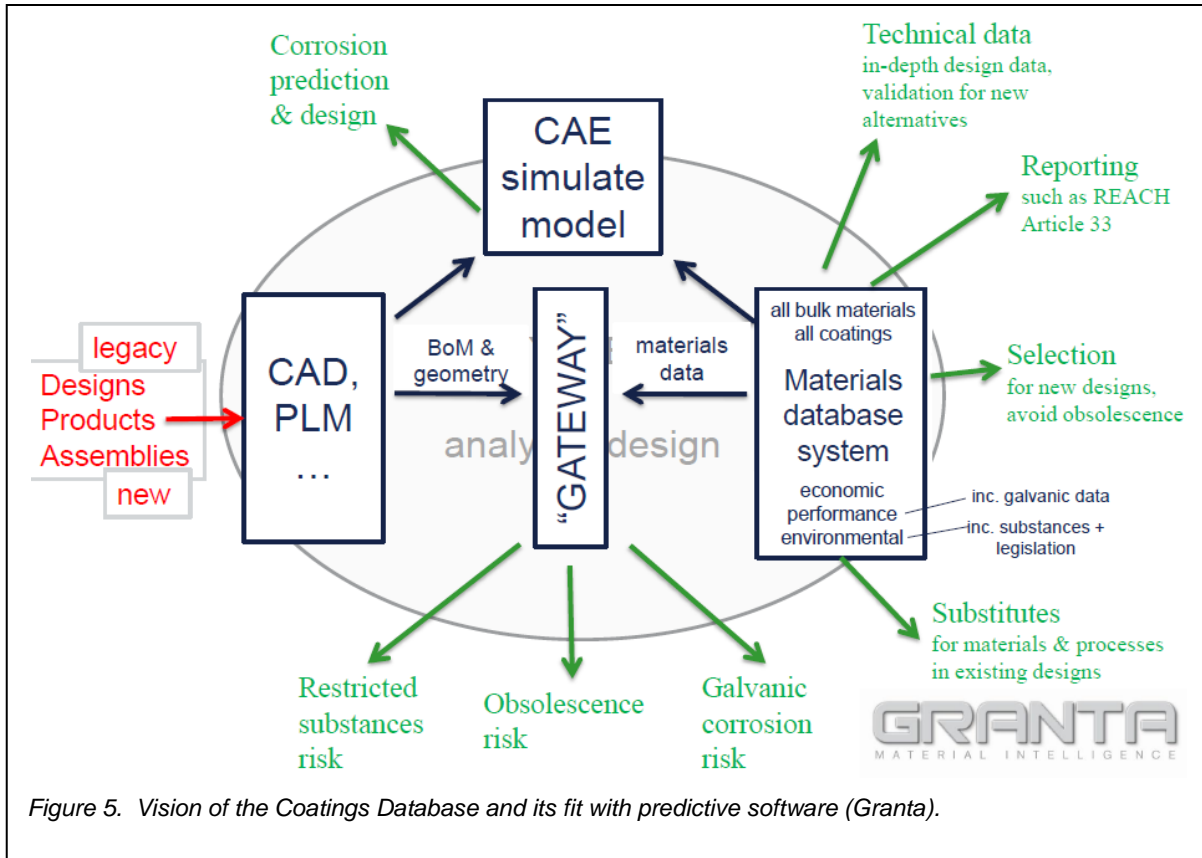
2.4. Coatings Databases (Patrick Coulter and Will Martin, Granta Design)

As the galvanic modeling shows, protection of corrosion rates requires a good database of coating properties and performance, including polarization curves. At the same time however it is also necessary for materials and coatings to comply with the various environmental and health regulations, including the European REACH regulations and the DoD memo on Minimizing the Use Hexavalent Chromium.

Granta described a Coatings Database (illustrated in Figure 5) based on their widely used Granta MI Materials Information system, that includes the following:

- Property data for a wide range of aerospace and defense coatings (hardness, adhesion, etc.)
- Performance data for coated materials (corrosion, fatigue, etc.)
- Chemistry of the coatings, including the CAS numbers of constituents, with an emphasis on SVHCs and

- other restricted substances
- Chemistry of the deposition processes (solutions etc,) including the CAS numbers of constituents, with an emphasis on SVHCs and other restricted substances
- Substitutes for coatings containing restricted materials (such as Cd, Cr⁶⁺, etc.)
- Coating galvanic potentials (but not yet polarization curves)
- Coating cost data, broken down by materials, labor, environmental cost, energy cost.



In addition to the database, Granta has developed a “Materials Gateway” to feed data, such as polarization curves, from the database to modeling software.

2.5. Galvanic Data Acquisition (Dennis Dull, Boeing)

Reliable and consistent galvanic data must be obtained to provide the polarization curves needed to feed into software such as that developed by Elsyca. Dennis pointed out that the standard galvanic table that is most widely used is a table of alloy galvanic potentials in flowing seawater that was developed about half a century ago. This means that it is not a reliable data set for most galvanic applications, which are frequently in quiescent rather than flowing water. It contains only ranges of galvanic potentials, rather than polarization curves, and it does not contain any of the new materials and coatings such as ZnNi.

What we need in order to accurately predict and design with galvanic data is polarization curves, corrosion rates, etc. all acquired using test methodologies and test conditions that are well defined and agreed-upon, consistent, and reproducible from one laboratory to another.

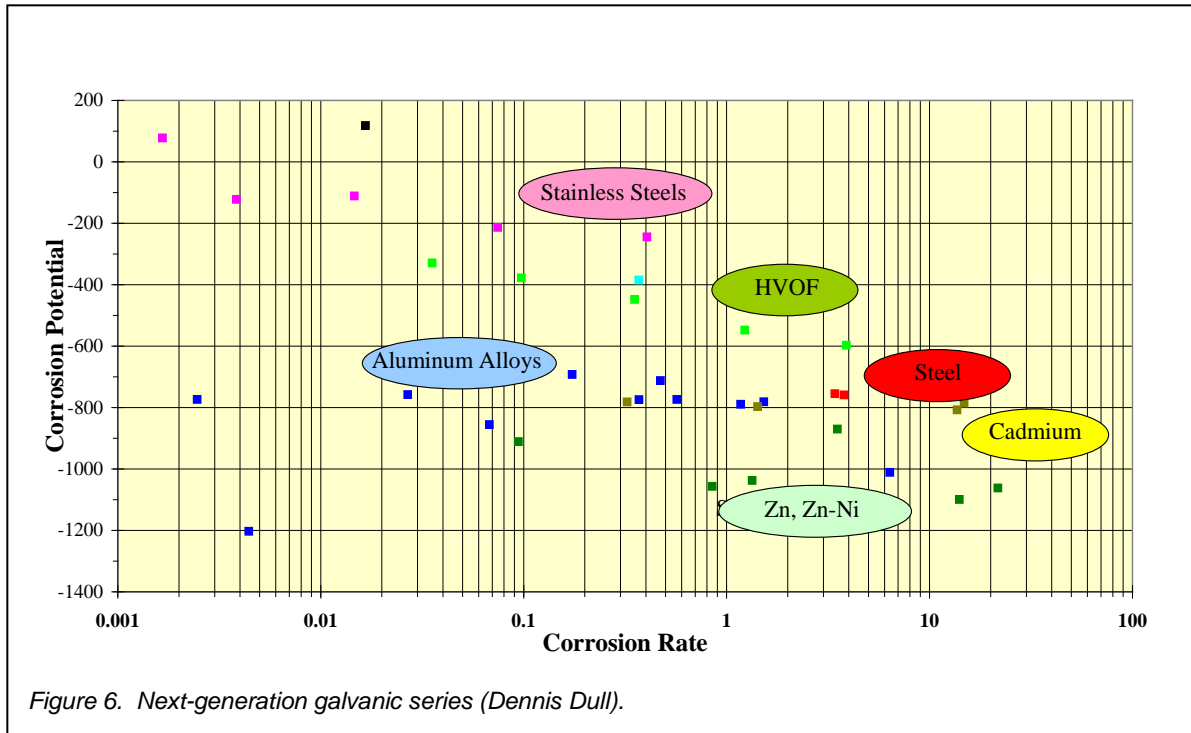
- What we do already—
 - Use “Galvanic Series”
 - Qualitatively rely on “tribal knowledge” & handbooks
 - Conduct laboratory tests
- What we want to do—
 - Use engineering tools to propose engineering solutions
 - Design tools require quantitative data
 - Quantify severity of corrosion on all geometries
 - Coupling between substrate of detail part and its finish (coating)

- Coupling of detailed parts of different materials
- Reduce/Eliminate Laboratory Tests

Boeing has been acquiring galvanic data in several forms:

- Steady-state Corrosion Potentials
- Steady-state Corrosion Rates
- Polarization Curves
- Initiated Next Generation Galvanic Series

Dennis proposed a next-generation galvanic table that would include both corrosion potential and corrosion rate (see Figure 6). This table contains alloys and coatings, including chromate conversion coatings, and shows how the corrosion potential and the corrosion rate depend upon the material and surface treatment.



2.6. cWorks (Steve Gaydos, Boeing)

For the C-17 program Boeing developed a methodology and associated software called cWorks for understanding and controlling the corrosion probability of components throughout the system. This methodology entailed groups of engineers getting together to discuss and agree upon the relative corrosion susceptibilities of different materials, coatings and components under different corrosion scenarios. The methodology attempts to capture the knowledge base of Boeing's corrosion experts and reduce it to a Relative Corrosion Index (RCI) for each component that can be used to improve design and to assign inspection intervals for each subsystem. The software also makes it possible to assess the relative risk of corrosion and decide whether any particular subsystem must be changed to lower the risk of corrosion. A patent for this methodology (Pat # 7,704,371) was issued in 2010.

The software incorporates three types of environmental - chemical attack:

- Environmental Attack of the Organic Surface Finish
 - Salt Spray
 - Anti-ice
 - Blue Water
 - UV
- Organic Surface Finish Damage
 - Sand
 - Gravel
 - Engine Exhaust
 - Maintenance
- Environmental Attack of the Parent Material
 - Salt Spray
 - Anti-ice
 - Blue Water
 - UV

Figure 7 shows the output from the cWorks software for the various components of an aircraft wing.

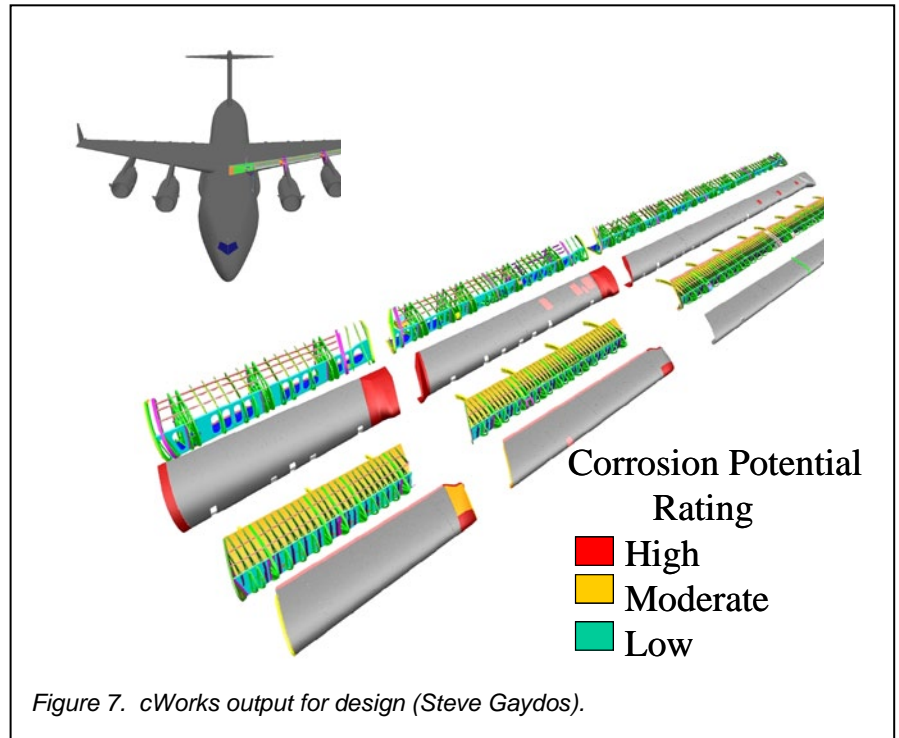


Figure 7. cWorks output for design (Steve Gaydos).

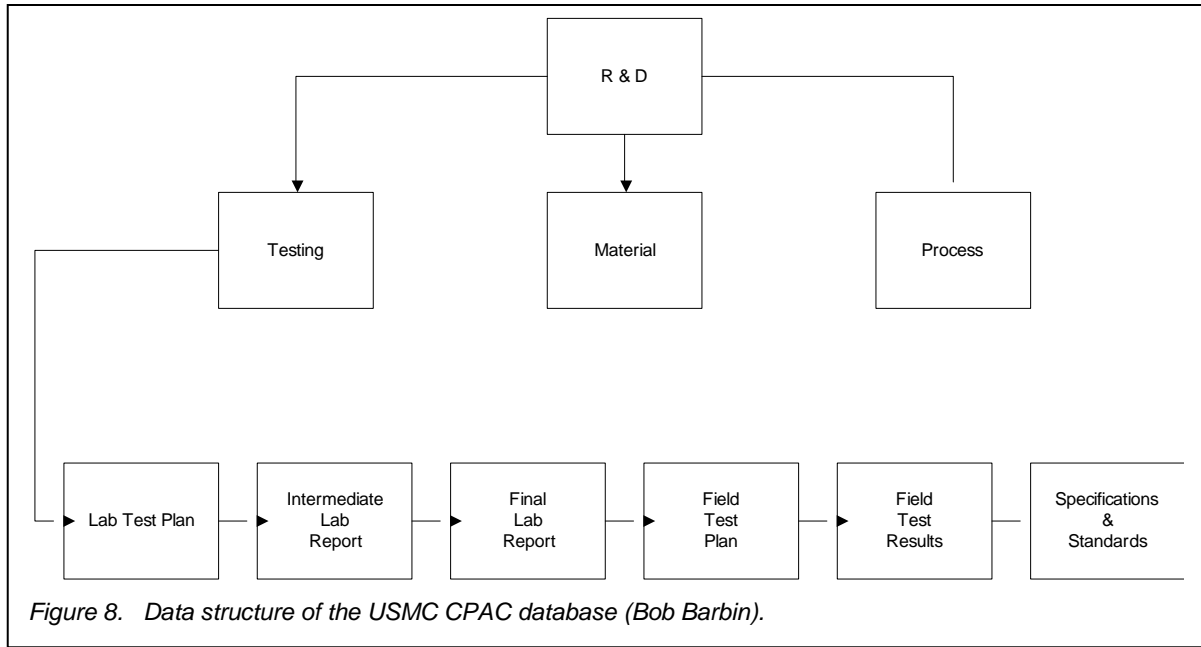
2.7. Corrosion Prevention and Control Database (Bob Barbin, Matt Koch, USMC CPAC)

One critical aspect of building more corrosion resistant weapons systems is capturing and making available to specifiers and designers the knowledge base on what works and what fails in current and legacy systems. The role of the US Marine Corps Corrosion Prevention and Control Program is to minimize corrosion in Marine Corps vehicles. A critical part of minimizing corrosion is capturing corrosion problems on existing systems to ensure that the same problems are not propagated to new systems, and to provide a knowledge base to assist maintainers in remedying corrosion problems on fielded systems. The USMC Corrosion Prevention and Control (CPAC) program is assembling a database as a comprehensive document repository of all CPAC-generated deliverables

- USMC and Joint-Service Acquisition Systems – Corrosion Prevention Control Plan (CPCP) and the full supporting documentation
- Research & Development to support
 - Acquisition Systems
 - Maintenance personnel
 - Depot Level: MCLBs (Albany and Barstow)
 - Middle Level: Corrosion Repair Facilities (CRFs)
 - Field Level: Corrosion Service Teams (CSTs)
 - DoD-wide applications (OSD Research projects)

The CPAC database will be joined with the ASETSDefense Surface Engineering Database (SED) to present program managers and designers with additional information with which to make their design and implementation decisions, in the light of increasing emphasis on environmentally acceptable coatings and treatments.

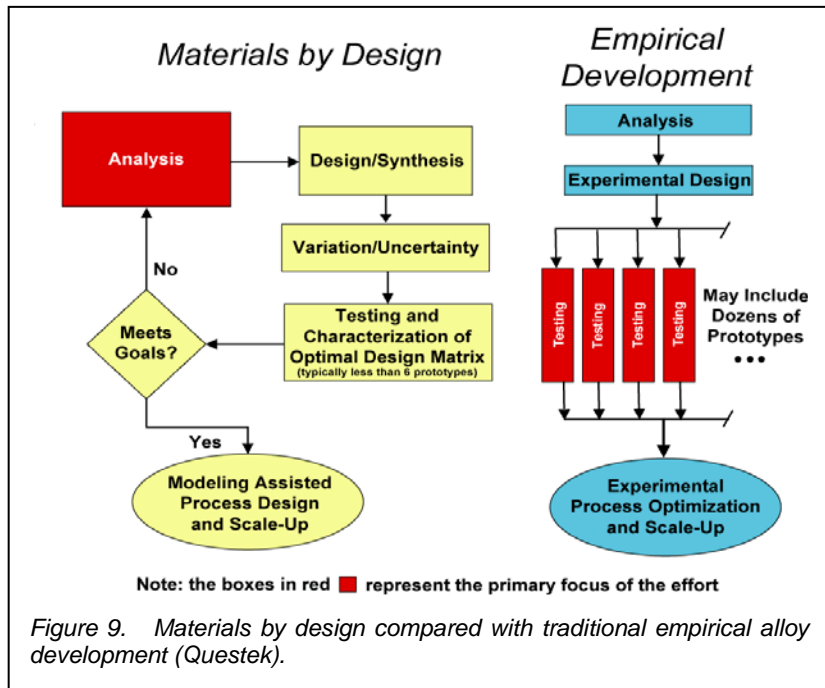
The database will provide access to the full documentation and testing history of a research project, as it pertains to CPAC (see Figure 8), as well as findings and recommendations from vehicle inspections. The link with the ASETSDefense database will provide engineering information on alternatives to chrome plated, cadmium plated, hexavalent chromium containing, and high VOC materials.



2.8. Materials by Design (Charles Kuehmann, Questek Innovations)

Over the past few years materials design has matured to the point where it is possible to design materials by computational methods. This approach can accelerate the design and qualification of a new material from a decade or more to a few years. In traditional empirical alloy development the bulk of the effort is in reformulating retesting material, whereas in Materials by Design the primary effort is in the up-front analysis, followed by relatively minor modifications and retesting (see Figure 9).

Once material has been designed by these computational methods qualification is easy since experimental data can be supplemented with computational predictions through an approach called Accelerated Insertion of Materials (AIM).



The Materials by Design and AIM approach has been demonstrated and validated in an ESTCP program to develop a new corrosion resistant ultrahigh strength landing gear steel, now commercially available as Carpenter S53.

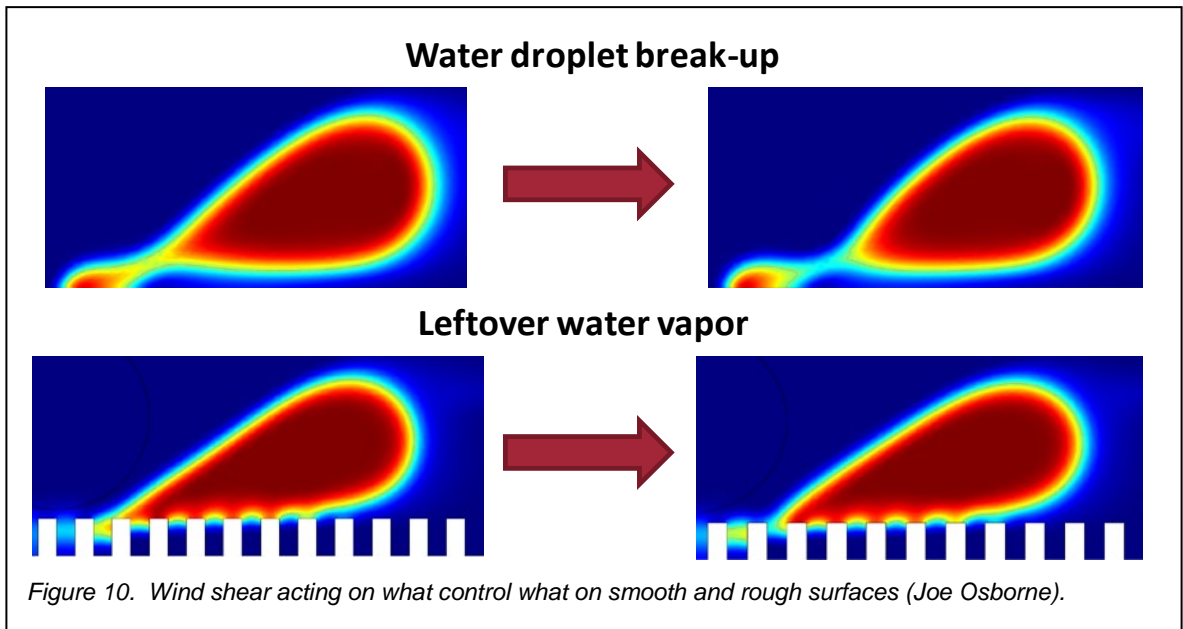
2.9. Atoms to Airplanes, the Future (Joe Osborne, Boeing)

In concert with Washington State University, Boeing is developing tools, methods, and an understanding of important parameters at the nano and micro level that govern macroscopic performance properties. The idea is to develop models and understanding beginning with the length and time scales of atomistic models, and extending them to predict the behavior of macroscopic systems. This approach was illustrated by a discussion of hydrophobic, anti-icing coatings including modeling of windshear for removing water droplets from surfaces, and modeling of corrosion and pitting.

The purpose of Atoms to Airplanes is understanding of processes at the atomic and molecular scale that can lead to more efficient materials development and product designs

- Gain insight into processes that are not otherwise measurable
- Augment lifetime prediction models based on test data and experience
- Understand interaction of materials with operational environment
 - Modeling tools are being developed to bridge length and time scales
- Taking advantage of increasing computing capability and algorithm developments
- Predictive capability is improving

For example, adhesion of water droplets onto flight surfaces can lead to icing. What is required is a surface that is hydrophobic and readily releases water droplets by windshear as the aircraft flies. Molecular dynamics modeling has been used to evaluate the hydrophobicity of materials, while finite element modeling has led to a better understanding of how droplets can be blown from the surface, and had their release can be improved by the use of microscale surface roughness (see Figure 10).



3. Summary

The ONR and NAVAIR programs (Design Modules for Corrosion Protection, and Durable Aircraft, respectively) have laid out a vision for integrating computational predictive corrosion modeling with design software. This vision would combine galvanic corrosion data with corrosion modeling to design weapons systems that are less corrosion-prone, minimizing the need for maintenance and reducing fleet lifecycle corrosion costs. This vision would begin with relatively simple steps, eventually allowing us to model and predict corrosion, including the full complexity of the system, the effects of corrosion products, and the different environments in which weapons system operate.

Although we have a long way to go to develop all the tools we will need to fulfill this vision, we have nevertheless reached a point where we do have useful tools that can be used to improve the performance of systems in the real world. We now have important parts of the toolset either completed or under development by organizations in different countries:

- 1. Databases of material properties and system performance**
 - a. Alloys and other materials, now including coatings, together with SVHCs and other restricted substances. This database system includes a Materials Gateway to feed data to computational models (Granta MI, Granta Design, UK).
 - b. Document encapsulating engineering experience and solutions for corrosion of weapons systems (CPAC Database, USMC CPAC).
- 2. Predictive models that span the range of models, from underlying science through computational electrochemistry to engineering experience**
 - a. Early development of modeling based on atomistic computations (Atoms to Airplanes, Boeing).
 - b. Predictive galvanic corrosion modeling software that integrates with CAD drawings (Galvanic Master, Elsyca, Belgium).
 - c. Predictive corrosion modeling and design software based on a formalized system of engineering experience (cWorks, Boeing).
- 3. Materials development models**
 - a. Materials by Design for rapid development and validation of alloys and other materials. This approach has not yet been applied to coatings and surface treatments, but there appear to be ways this might be done (Questek Innovations, USA).
- 4. New galvanic corrosion measurement methodology and dataset**
 - a. A consistent methodology for acquiring galvanic corrosion data suitable for use in computational modeling; this includes the development of new galvanic tables that will incorporate all of the modern materials, coatings, and surface treatments (Boeing).

In the immediate future the use of databases that capture system and component performance (such as those of USMC and Boeing) will ensure that lessons learned on today's systems are not lost.

In the short term the combination of polarization curves held in a standard database, with predictive galvanic modeling will suffice to begin ONR's Design Modules for Corrosion Protection. In order to realize NAVAIR's Durable Aircraft vision the database of galvanic and performance data for materials, coatings, and surface treatments will need to be expanded, building in effects such as the service environment, protective system damage, and the products of corrosion itself. With the growth in recent years in the number of structural materials, coatings and treatments, a consistent, reliable, and comprehensive database of materials properties, especially galvanic performance, will be essential.

Given the compressed timescales that are driving environmental substitution, we will need to develop rapid design, qualification, and implementation of new materials and coatings, without compromising safety or performance. Computational design tools have already been demonstrated for alloys, but not yet for coatings. Efforts are underway to develop rapid testing methods, especially for corrosion, as discussed in briefings presented elsewhere in the ASETSDefense 2011 Workshop.

In the long run a basic science approach will be required to develop better materials and understand what controls the performance, including chemistry, structure and morphology.