Integrated Computational Materials Engineering: A Study on Implementing ICME in the Aerospace, Automotive & Maritime Industries

Tresa Pollock
University of California, Santa Barbara

George Spanos
The Minerals, Metals & Materials Society
Full Project Team

• TMS Staff: Project lead, facilitate project team work, final report, dissemination and promotion

• Nexight Group (LLC): Facilitate project team work, work with TMS on final report

• ICME Implementation Teams (IITs): Subject matter experts
  - Responsible for the content of this work
  - The “brains” & experience behind this study
Team Leaders
Tresa Pollock (U. of California - S.B.)
John Allison (U. of Michigan)
John Deloach (Naval Surface Warfare Center)
Brad Cowles (Pratt & Witney - retired)
Justin Scott (TMS)

TMS Leads
Project Leader (PI): George Spanos
Project Coordinator: David Howe

Funding Support
DoD (ONR, AFRL), DOE, NSF
Motivation

- Support ICME & MGI goals of accelerating development (at reduced cost) of advanced materials and manufacturing processes: from discovery to deployment

- ICME recognized as new discipline & awareness growing worldwide
  - 2008 National Academies report established ICME as a discipline, overall vision, discussed broad cultural & technical issues
  - ICME World Congress(es), Journal issues, books, courses/workshops, etc.

- Although some ICME case studies to date, to realize this vision more extensively, and rapidly, a focused study was undertaken to define the frameworks and pathways to **ICME implementation in the near term (≤ 3 yrs.)**
Some Background

• 14 Month Study: June, 2012 - July, 2013

• Centered predominantly on lightweighting (and propulsion) applications in three industrial sectors


• Study results and report will be rolled out at “The 2nd World Congress on ICME” July 7, 2013 in Salt Lake City, Utah
Overall Project Goals/Tasks

• Recommendations for ICME implementation in aerospace, automotive, and maritime industrial sectors
  • “Field manual” for practitioners to implement ICME

• Develop “Frameworks” for ICME Implementation
  • Steps, computational tools, experiments, people, flow of information/data - across product development cycle

• Implementation time frame: next 1-3 years to begin an ICME-accelerated product development program

• Report could nucleate self-assembly of ICME teams and/or programs
Project Overview

• Five ICME Implementation Teams
  - 3 teams, each associated with a specific industry
  - 4th team - pervasive cross cutting issues
    - e.g.: verification/validation, uncertainty quantification, integrating design ....
  - 5th team: review panel for final report

• 1st three teams:
  - Aerospace industry
  - Automotive industry
  - Maritime industry
ICME Implementation Teams

• Composition of each team:
  • Team leader
  • ~ 10 top technical experts:
    - ICME, materials, design, engineering, applications
    - variety of materials types (metals, composites, ceramics)
    - majority industry; key academics and gov. as well

• Team mechanics:
  • Series of on-line meetings
  • “Homework” assignments to support meetings
  • Two-day in-person facilitated working sessions for each of four teams
  • Iterative editing on final report
Team Leaders

• **Aerospace**: Tresa Pollock  
  - Univ. of Cal. at Santa Barbara - Dept. head  
  - Chair of 2008 National Academies study on ICME

• **Automotive**: John Allison  
  - Univ. of Michigan Professor (much of career at Ford)  
  - Co-Chair of 2008 National Academies study

• **Maritime**: John Deloach  
  - Naval Surface Warfare Ctr - Welding Branch Head (& ONR)  
  - Handles many materials issues for Navy platforms

• **Crosscutting**: Brad Cowles  
  - Consultant - retired Pratt & Whitney (37 years)  
  - Oversaw tech. projects & technology development programs

• **Report Review**: Justin Scott  
  - TMS Technical Project Leader  
  - Worked on ICME-related studies at Inst. for Defense Analysis
ICME Implementation Teams
By Affiliations

### Aerospace
- University of California - S. B.
- Cowles Consulting / Pratt&Whitney
- GE-GRC
- GE Aviation
- AFRL
- Lockheed Martin
- Pratt & Whitney
- Boeing
- Boeing

### Automotive
- University of Michigan
- Timken
- Hydro Aluminum
- Ford
- GM
- University of British Columbia
- Pacific Northwest National Lab.
- Consultant
- Alcoa

### Maritime
- Naval Surface Warfare Center
- EWI
- Ingalls Shipbuilding
- Naval Surface Warfare Center
- Arcelor Mittal
- Naval Research Laboratory
- Office of the Secretary of Defense (OSD)
- HII-Newport News
- NAVSEA

### Cross-Cutting
- Cowles Consulting / Pratt&Whitey
- Thermocalc
- Georgia Tech.
- Pratt & Whitney
- Alcoa
- Purdue
- ESI
- University of Oklahoma
- Northwestern
- University/Questek

### Review
- TMS
- Naval Research Laboratory
- University of North Texas
- NIST
- General Electric (retired)
- General Motors
- Oak Ridge National Lab.
- University of Michigan
- Tinken Steel

* Mixture of Big Industry, Smaller Companies, Academia, Government*
ICME Implementation Study
Status Update

Task 1: Recruit ICME Implementation Teams
(teams & virtual groups)
Task 2: Prepare Teams
(research, conf. calls, etc.)
Task 3: Convene Individual Teams
(working meetings)
Task 4: Prepare Report
(iterate with teams)
Task 5: Disseminate/Communicate
(project status & report)

On course for release at ICME 2nd World Congress in July

Task 1 - complete
Task 2 - complete
Task 3 - complete
Task 4 - in progress (draft in review)
Task 5 - in progress (press releases, TMS e-news, JOM, etc. to date)
Study Outputs (For Report)

- “Frameworks” detailing steps needed to execute an ICME-Accelerated Product Development Program (IAPDP) in each industrial sector
- Current state of ICME Implementation
- Detailed actions at each step within IAPDPs, for each of the three frameworks
- Descriptions of personnel needed for each step in an IAPDP
- Detailed strategies for addressing needs & barriers to ICME implementation in near term (1 - 3 yrs.)
- Recommendations for more than 50 application opportunities for Implementing ICME in near term
- Critical pervasive, crosscutting issues and recommendations
ICME Models and Toolsets: **Key** for shapes in blue above

- Suites of models are identified or developed (8, 12, 16)
- Models are validated and verified [V&V’d] in iterative processes (9, 13, 17)
- Linking tools transmit data between models (11, 15, 19)
- Suites of V&V’d computational tools are applied to the specific product development (10, 14, 18)
• This specific framework is for **Automotive** industry
• This particular overlay includes types of *personnel* needed at each step
• Highlight: provides location and interactions of various personnel types at various steps in the Integrated Product Development Cycle
  - E.g., design & release engineer, manufacturing engineer, research experimentalist, materials engineer, production analyst, ICME expert/integrator....
This specific ICME toolset portion of a framework is from the Maritime industry chapter.

Overlay here highlights examples of some of the computational & experimental tools employed at each step in the ICME toolset.

E.g., ABAQUAS, ThermoCalc, ProCAST, SysWeld, Gleeble .....

- 8 V&V'd Models to Predict Processing Outcomes
  - Assess and use a suite of modeling tools to predict the processing outcomes.
  - Typical computational codes to include:
    - Gleeble: Used to obtain stress-strain-microstructure relationship linked to processing (e.g., hot rolling)
    - ABAQUAS: Standard FEM stress/strain prediction analysis used for general modeling of forging
    - MSC/NASTRAN: Standard FEM stress/strain prediction analysis used for general modeling of forging
    - ProCAST/QuaICAST: Cast design with processing
    - MAGMASOFT: Cast design
    - SysWeld: Simulation and design optimization of heat treatment, welding, and welding assembly
    - Weld Planner: Simulation and design optimization of heat treatment, welding, and welding assembly

- 10 Suite of Modeling Tools to Predict Microstructure
  - Assess and use a suite of models to predict the microstructure (or other length scale structure) of the material.
  - Typical computational codes to include:
    - Thermo-Calc: CALPHAD method-based software; thermodynamic and phase diagram calculations
    - VRC/CAST/VRIFAB/VRIFORM: As-cast microstructure modeling of grain size/growth/morphology and precipitation physics prediction; used for microstructure and property prediction

- 11 V&V'd by Experiment

- 12 V&V'd Models to Predict Microstructure

- 14 Suite of Modeling Tools to Predict Mats/Component Properties

- 15 V&V'd by Experiment

- 16 V&V'd Models to Predict Materials/Component Properties
  - Assess and use a suite of models to predict materials properties.
  - Typical computational codes to include:
    - Gleeble: Used to obtain the stress-strain-microstructure relationship associated with the processing of the material (e.g., hot rolling)
    - VRC/CAST/VRIFAB/VRIFORM: As-cast microstructure modeling of grain size/growth/morphology and precipitation physics prediction; used for both microstructure and property prediction
    - BEASY: Simulation of corrosion phenomena, and crack growth associated with corrosion

- 17 Linking Tools
**ICME Implementation Study Report**

**A Field Manual for Implementing ICME in the Aerospace, Automotive, and Maritime Industries**

- Detailed table entries corresponding to different steps in the frameworks – one example from **Aerospace** chapter draft

<table>
<thead>
<tr>
<th>Step</th>
<th>Actions and Tools</th>
</tr>
</thead>
<tbody>
<tr>
<td>17. Decision Point: Verify and validate models using experimental tools</td>
<td>- Conduct series of experiments to validate that the modeling results are representative of real-world conditions and design experiments specifically to work within the bounds of the model to confirm validity. Experimental tests could include:&lt;br&gt;  - <em>Experiments to validate the thermodynamics (phase diagram) results, which could include:</em>&lt;br&gt;    - Heat treatments (isothermal and/or continuous cooling)&lt;br&gt;    - Microscopy: Optical microscopy, SEM/EBSD, and/or TEM to characterize microconstituents resulting from the heat treatments.&lt;br&gt;    - Differential Thermal Analysis (DTA)&lt;br&gt;  - <em>Experiments to measure mechanical or other physical or thermo-physical properties (including output of ANSYS), which could include:</em>&lt;br&gt;    - Neutron diffraction (residual stress)&lt;br&gt;    - X-ray diffraction techniques&lt;br&gt;    - Creep testing (engine components)&lt;br&gt;    - Corrosion testing&lt;br&gt;    - Tensile tests (yield and ultimate strength, ductility – elongation/reduction in area).&lt;br&gt; - Conduct series of tests to verify the computational accuracy of the modeling software and confirm that any physics-based codes are correctly executed.&lt;br&gt;  - Note: This may require several iterations of experiments or adjustments to the modeling tools ensure validity.</td>
</tr>
</tbody>
</table>

- See next two slides for some details >>>>>>
### ICME Implementation Study Report
A Field Manual for Implementing ICME in the Aerospace, Automotive, and Maritime Industries

<table>
<thead>
<tr>
<th>Step</th>
<th>Actions and Tools</th>
</tr>
</thead>
</table>
| 17. Decision Point: Verify and validate models using experimental tools | - Conduct series of experiments to validate that modeling results are representative of real-world conditions and design experiments specifically to work within bounds of model to confirm validity.  
  - Experimental tests could include:  
    - Experiments to validate the thermodynamics (phase diagram) results, could include:  
      - Heat treatments (isothermal; continuous cooling)  
      - Optical microscopy, SEM/EBSD, and TEM to characterize microconstituents resulting from the heat treatments  
      - Differential Thermal Analysis (DTA) |
### Step 17. Decision Point: Verify and validate models using experimental tools

<table>
<thead>
<tr>
<th>Actions and Tools</th>
</tr>
</thead>
<tbody>
<tr>
<td>- <em>Experiments to measure mechanical, physical, properties (including output of ANSYS); could include:</em></td>
</tr>
<tr>
<td>- Neutron diffraction (residual stress)</td>
</tr>
<tr>
<td>- X-ray diffraction</td>
</tr>
<tr>
<td>- Creep testing (engine components)</td>
</tr>
<tr>
<td>- Corrosion testing</td>
</tr>
<tr>
<td>- Tensile tests (yield and ultimate strength, ductility – elongation/reduction in area)</td>
</tr>
</tbody>
</table>
Excerpts from Maritime chapter draft

<table>
<thead>
<tr>
<th>Step</th>
<th>Actions and Tools</th>
</tr>
</thead>
</table>
| 5. Material Composition | - Conduct research to investigate materials candidates and alloy compositions…. include extensive literature review  
- Utilize computational codes such as Thermocalc or Pandat to help determine potential materials compositions  
- Examine compositional design options using set of trials and screening options on small-scale components (e.g., plates or filler wire). |
### Excerpts from *Maritime* chapter draft

<table>
<thead>
<tr>
<th>Step</th>
<th>Actions and Tools</th>
</tr>
</thead>
</table>
| 5. Material Composition | • Define and complete experimental test matrix to down-select to preferred materials compositions and processing approach  
  • Make changes/additions to fabrication specifications using performance requirements, geometry, matls. composition  
  - *Note: From this point through step 26, the materials suppliers are driving the process with metallurgical knowledge, etc.* |
Who Should Read This Report and Why?

- A variety of stakeholders (or potential stakeholders) throughout various organizations, including:
  - Professionals in aerospace, automotive, & maritime industries
  - People in other materials-intensive industries
  - University professionals and students
  - Government scientists and engineers, program officers, and policy makers

- Report discusses not only who should read it, but:
  - Why, and what benefits they will receive
  - What actions they might take after reading this report
  - Can be read at different “resolutions”, depending on level of previous involvement in ICME or product development
    - Some take a deep, full read
    - Others - executive summary (~8 pages), final comments, and skim text
Creating a Business Case for ICME

- Need: convincing stakeholders to adopt ICME methods:
  - Modeling software, supporting databases, and qualified personnel are significant investments
  - Often viewed as a substantial business risk from the perspective of management
  - Want to ensure they achieve their expected return on investment (ROI)
  - Others…….

- Recommended Actions
  - Develop a quantitative economic case
  - Document case studies and lessons learned
  - Address risk and uncertainty quantification and mitigation
  - Others…….
One Example

Detailed Tactics for one of these recommended actions

• **Develop a Quantitative Economic Case**
  • Provide a sound *quantitative analysis* that details the benefits
  • Specifically, define how an ICME-accelerated product development cycle can reduce risks, costs, and/or time expenditures
  • Contributions to such reductions include decreased testing requirements; reduced risk, time, and iterations for materials and process development
  • Elimination or reduction of costly traditional product iterations
  • Consider the *complete manufacturing chain* of a particular material or component rather than just the cost of the raw material, and demonstrate reduced cost or time expenditures
  • Etc….
Strategies for addressing needs & barriers to ICME implementation in the near term (1 - 3 yrs.) – one example from the draft report

• Needs
  o Improved Quantitative Modeling Tools, Including:
    ➢ Microstructure model tools for high-pressure die casting aluminum & magnesium alloys
    ➢ Tools to predict forming/welding induced property changes in subsequent crash and noise-vibration-harshness simulation
    ➢ Others….

• Recommended Actions
  o Two-day workshop with representatives from industry and academia (and publish results)
  o Establish best practices for evaluating maturity and predictive capability of different software tools and models
  o Others….
Concluding Remarks - 1

• It is a very exciting time in Matls. Sci. & Engineering

• In large part due to application of MS&E innovations into industry to develop advanced new products – ICME

• ICME now recognized as a discipline, worldwide awareness is growing rapidly, leveraged with MGI

• Great potential for ICME to reduce significantly time & cost of developing materials, components, and manufacturing processes

• But we stand at a critical juncture or “tipping point”
Concluding Remarks - 2

• To realize this vision, we need detailed pathways to rapid implementation

• We all have some part to play in the success of ICME

• This study considered a “field manual” for near term ICME implementation

• Provides practioners with
  - frameworks, recommended actions & personnel, near term opportunities to imbed ICME into product development cycles within ~ 3 years

• Final report to be first published and distributed on July 7, 2013 (at 2\textsuperscript{nd} World Congress on ICME)
Thank You!

Questions