Clean Energy Technologies: Growing Need for Multiphysics Modeling

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SRI headquarters, Menlo Park, CA



Sarnoff headquarters, Princeton, NJ

SRI International

- Independent R&D organization
- Founded by Stanford University in 1946
 - A nonprofit corporation
 - Independent in 1970; changed name from
 - Stanford Research Institute to SRI International in 1977
- Sarnoff Corporation acquired in 1987 (formerly RCA Laboratories)
- 2,000 staff members combined
 - 800 with advanced degrees
 - More than 20 locations worldwide
- Consolidated 2007 revenue: \$450 million



SRI State College, PA



SRI Tokyo, Japan



SRI Washington, D.C.



What we do



- Customer-sponsored R&D
 From discovery, study, and evaluation to custom solutions on demand
- Licenses

Innovative technologies ready for use

- Ventures
 - Spin-off companies to capitalize on new opportunities
- Innovation partnerships



A Foreword on Clean Energy Ostwald* wrote in 1894:

- The way in which the greatest of all industrial problems that of providing cheap energy is to be solved, must be found by electrochemistry.
- Once we have an electrochemical cell that yields electricity direct from coal and air, then we stand on the threshold of an industrial revolution that will dwarf the one that followed upon the invention of the steam engine



Energy Generation in the US





Efficiency Limits

Thermodynamic efficiency of a fuel cell: $\eta_t = \frac{\Delta G}{\Delta H} = 1 - \frac{T\Delta S}{\Delta H}$





System and Model



Technical Approach





DCFC concept with liquid anode carrying solid fuel.

DCFC fuel element.

- DCFC generates electricity by the electrochemical oxidation of carbon atoms by O²⁻ ions with the release of four electrons and a CO₂ molecule
- The fuel oxidation reaction takes place at the interface of the liquid anode and solid electrolyte or in the bulk of the liquid anode
- Oxygen ions are generated from oxygen molecules by the solid cathode on the opposite side of the electrolyte and migrate through the electrolyte to the fuel oxidation zone.
- Unique combination of high (>70%) efficiency of energy conversion and the high energy density
 of carbon fuel (20 kW-hr/l)
- Tubular elements are obtained from SOFC industrial manufacturer (without solid gas diffusion anode)



Beginning: Nature Inspired Algorithm

- Problem: come up with molten salt circulation concept
- Approach: try COMSOL trial version over a rainy weekend
- Output: qualitative picture of molten salt velocity field in a day (Newton, 2D, single phase)
- Decision: get COMSOL license
- Finally: bi-directional coupling of wishful thinking and reality in the lab









DCFC Modeling at SRI



Summary

- Multi-physics and multi-scale
- Seamless coupling is vital
- Resources management
 - Symmetry
 - Integral models
- Version 3.5
 - Geometry parameterization
 - Sensitivity analysis
- THANK YOU:
 - COMSOL in general and PALO ALTO OFFICE in particular

