Modeling and Simulation
SECA Core Program

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Integration Meeting

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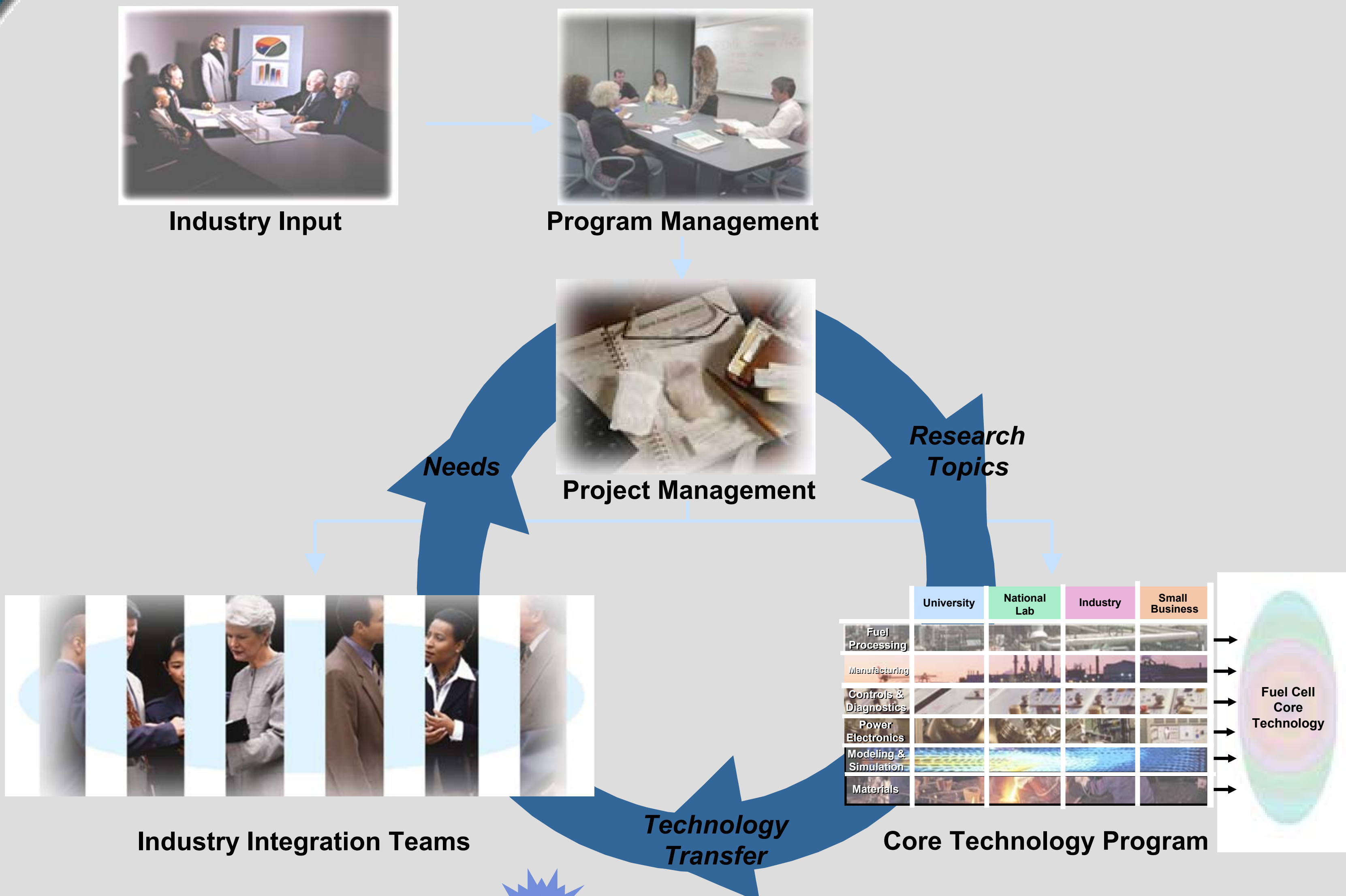
Battelle

NETL

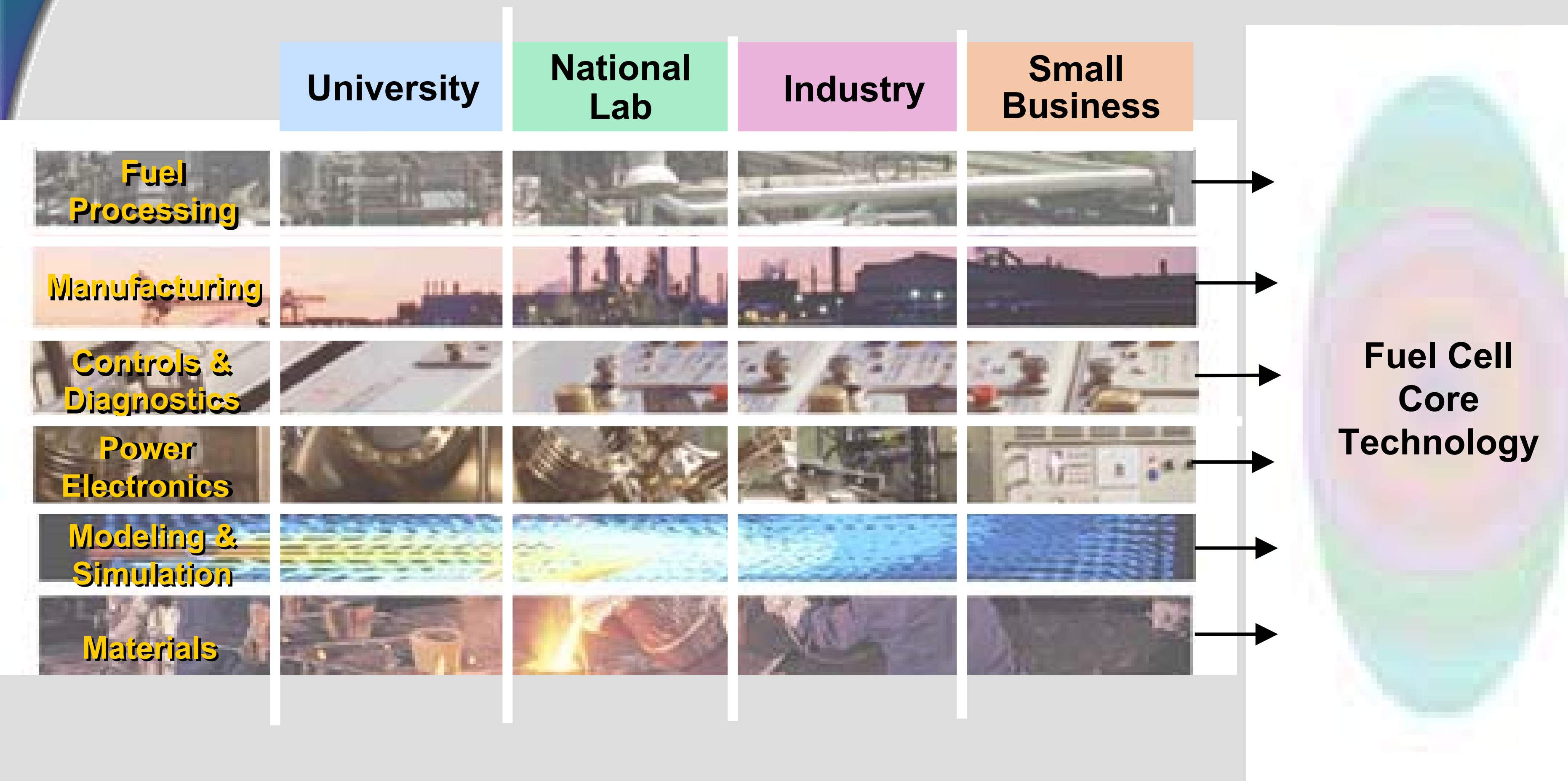
Pacific Northwest National Laboratory

Operated by Battelle for the U.S. Department of Energy

SECA Program Structure



Core Technology Program
The Technology Base



System Analysis : Overall System Goals

- Evaluate overall system configuration
- Evaluate energy transfer and system efficiency
- Determine sub-system requirements
- Determine system performance at various loads
- Evaluate dynamic system performance during start-up
- Evaluate controller performance

System Analysis : Reformer Sub-System Goals

- Determine optimum fuel to air ratios
- Determine performance of different fuel compositions
- Evaluate heat transfer necessary for fuel vaporization

Stack Analysis :
Stack Sub-System Goals

- Stack design
  - Flow distribution
  - Pressure drops
  - Overall thermal characteristics
  - Stress and strain distribution
- Evaluate Stresses due to:
  - Manufacturing (residual stresses)
  - Differential thermal expansion
  - Temperature gradients
  - External mechanical loads
  - Oxygen activity gradient (MIEC materials)
- Evaluate stack initial electrochemical performance
- Stack structural and electrical reliability

Degradation

Component	Electrical Degradation	Mechanical Degradation
Interconnect	►Oxidation (resistance) ►Cr Volatization (Cathode) ►Migration of other species (contact materials)	►Loss of material due to oxidation ►Plastic deformation (thermal cycling)
Anode	► Ni sintering (decrease of TPB, increase anode resistance, wraping (electrical contact), restricted gas diffusion	►Ni sintering •Dimensional stability •Cracking within anode •Interfacial and failure cracking ►Damage due to thermal gradient and cycling
Cathode	►Suscetability to Cr poisonous ►Interfacial reaction (diffusion –e.g., Zr into ferrite, second phase at interface)	
Electrolyte	►Aging effects (σ vs t, phase stability)	►Damage due to thermal gradient & thermomechanical cycling
Seal	►Poisoning of electrode ►Electrical degradation due to seal failure at gas leakage	►Changes in thermal/ mechanical properties upon devitrification and subsequent high temperature operations ►Interfacial reactions ►Seal material stability and volatilization ►Seal material and interface degradation due to thermal gradients, cooling and cycling

Tools for SOFC system

Electrical Power System	▶Power/Energy versus Time ▶System dynamics modeling tools ▶System electrical design			
Thermal System		▶System thermal/ material flow ▶System thermal modeling tools ▶System thermal design		
Stack and manifolds			▶Rapid start-up (flow-thermal-stress) ▶Empirical electrochemistry tools and coupling with engineering codes ▶Steady state analysis ▶Concept evaluations	
Cell				▶Detailed electrochemistry models ▶Internal reformation ▶Cell concept evaluation

Modeling and Simulation

Current Status

- System modeling
  - Thermal system modeling using standard commercial codes for SOFCs with simplified stack and reformer sub-models. SECA core program participants developed a stack sub-model which was incorporated into ASPEN.
  - Models for steady state
  - Modular development
- Stack
  - Flow, thermal and stress commercial codes are available. Recently SECA core program participants incorporated a simplified electrochemistry routines. Engineering level simulation are needed for design and optimization.

Modeling and Simulation

Current Status (cont'd)

- Fundamental/Cell
  - Models for describing the polarization of the electrode due to interaction between electrochemical kinetic resistance, mass transfer resistance and ohmic resistance.
  - Models for describing the kinetics of the reactions at the interface between the electrode and electrolyte, the conduction process in the electrolyte and that in the electrode.
- Crosscutting
  - Limited data for input into engineering and electrochemical models
  - Limited data for validation on cell and cell components

Modeling and Simulation

System Needs

- Evaluate and select system modeling tools
  - Aspen, Simulink, Sabre, NPSS
- Enhance system models
  - Integrate more detailed component and stack models
  - Weight, volume estimation
- Transient/dynamic models
  - Load perturbations
- Electrical systems models
  - Inverters, regulators, generators
- Internal/external reformer
- Material, production, .. cost analysis models

Modeling and Simulation

Stack Needs

- Robust multi-physics stack models
- Compressive and rigid seals models
- Life prediction
  - Electrochemical and mechanical degradation
  - Enhancements to ICARES for fuel cell materials
- Fabrication warpage and residual stress models.

Fundamental cell needs

- Microstructural models
  - Microstructural design and optimization
  - Internal reforming
  - Electrode performance (short and long term)

Modeling and Simulation

Cross-cutting

- Thermo-mechanical data data appropriate for incorporation in engineering codes for fuel cell components:
  - Interconnect
  - Seals
  - Cell (after reduction)
- Fabrication defects (types, density) and relation to fabrication methods.
- Experiments for investigating degradation (electrical and mechanical)
- Model validation

System Electrochemistry and Cost Models

	Execl & Matlab Stack Model	Transient Models	PES	BOPS	Integration with other codes
Stack/ system	PNNL	UIC/VT/GT – Lagrangian Approach and superposition	Models based bifurication analysis (UIC/VT/GT)	UIC/VT/GT	UIC/VT/GT PNNL

	Model integration	Product Performance	Web-Based Interface
System	Manufacturing processes, materials (TIAX)	TIAX	TIAX

Stack & Cell Electrochemistry Models

	Empirical Electochemistry models	Integration with Engineering Codes	Button-Size Cell Coupon Experiments	1-cell or 3 cell verification
1-cell Stack	PNNL NETL	Fluent (NETL) STAR-CD (PNNL) MARC (PNNL)	PNNL (fabrication and testing) NETL (testing)	
Multiple cell Stack		STAR-CD (PNNL) MARC (PNNL)		PNNL (fabrication and testing)
Electrical Degradation		MARC (PNNL)		PNNL (testing and verification)

	Effective Property model	Discrete Particle	Defect Modeling
Cell	Lattice Boltzman & Chemkin or Surface Chemkin (PNNL)	Lattice Boltzman	U of F
Material			MIEC

Thermo-mechanical Models

	Constitutive Relations	Sub-models	Fabrication Models	Stack Models
Cell	Elastic properties as function of temperature and porosity (ORNL) Establish relations for code implementation (PNNL)	Tri-layer models and parametric studies (PNNL) Buckling driven delamination (GT) Fracture mechanics (GT) Data on type of defects (ORNL) Fracture toughness (ORNL) Creep models (PNNL and ORNL	Residual stress prediction (SNL) Wrapage prediction (SNL)	ICARES (ORNL)
Seal	Experiments (PNNL) Establish relations for code implementation (PNNL)	Leak models for mica seals		
Interconnect	Establish relations for code implementation (PNNL)			
Stack				Structural analysis in ANSYS or MARC (PNNL) ICARES (PNNL and ORNL)

Mechanical Experiments

	Elastic properties as function of temperature and porosity	biaxial strength at temperature	Fracture Toughness	Interfacial Toughness
Reduced Anode - Electrolyte	PNNL (fabricates materials) ORNL (testing)	ORNL(testing)	ORNL & GT	ORNL &GT
Tri-layer material				ORNL & GT

	Thermal Shock	Creep testing
Cell/frame **Cell/BC**	PNNL (fabricates and tests)	PNNL(testing)

	Elastic properties as function of temperature	Popgun test	Thermal cycling and leak testing
Glass Seal	PNNL (fabricates and tests)	PNNL(testing)	PNNL
Mica Seals	PNNL (frictional force versus normal load)		**PNNL**

Degradation

Plans

- Integrate the scope of work into a master plan.
- Leverage activities among the team.
- Logistics:
  - Each member will have 30 minutes to present on-going and planned activities.
  - SECA vertical team and other core team members will have 10 minutes for questions and answers after each talk.
- Don and I will follow up with each team member regarding the scope of work based on comments and feedback from this meeting.