Fuel Cells Systems Analysis

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Project ID: FC17

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Overview

Timeline

- Start date: Oct 2003
- End date: Open
- Percent complete: NA

Budget

- FY12 funding: $600K
  DOE share: 100%
- FY11 funding: $700K

Barriers

B. Cost

C. Performance

E. System Thermal and Water Management

F. Air Management

J. Startup and Shut-down Time, Energy/Transient Operation

Partners/Interactions

- Honeywell CEM+TWM projects
- SA
- 3M, Gore
- ISO-TC192 WG12, JARI, LANL
- IEA Annexes 22 and 26
- Transport Modeling Working Group
- U.S. DRIVE fuel cell tech team

- This project addresses system, stack and air management targets for efficiency, power density, specific power, transient response time, cold start-up time, start up and shut down energy

Objectives and Relevance

Develop a validated system model and use it to assess design-point, part-load and dynamic performance of automotive and stationary fuel cell systems.

- Support DOE in setting technical targets and directing component development
- Establish metrics for gauging progress of R&D projects
- Provide data and specifications to DOE projects on high-volume manufacturing cost estimation

Approach

Develop, document & make available versatile system design and analysis tools.

- GCtool: Stand-alone code on PC platform
- GCtool-Autonomie: Drive-cycle analysis of hybrid fuel cell systems

Validate the models against data obtained in laboratory and at Argonne’s Fuel Cell Test Facility.

- Collaborate with external organizations

Apply models to issues of current interest.

- Work with U.S. DRIVE Technical Teams
- Work with DOE contractors as requested by DOE

Collaborations

Air Management	Honeywell Turbo Technologies
Stack	3M, Nuvera
Water Management	Gore, Honeywell Aerospace, NJIT
Thermal Management	Honeywell Thermal Systems
Fuel Management	3M
Fuel Economy	ANL (Autonomie)
H_2 Impurities	JARI, LANL, ISO-TC-192 WG
System Cost	SA
Dissemination	IEA Annex 22 and 26, Transport Modeling Working Group

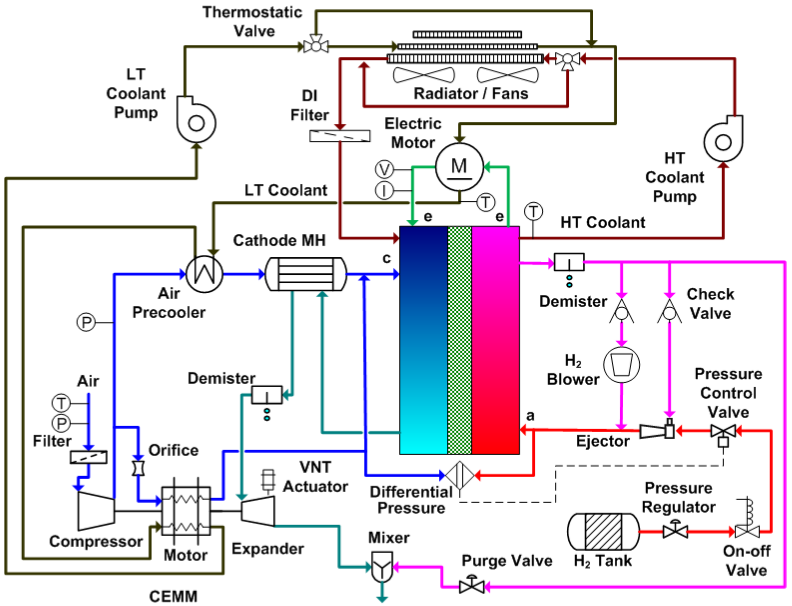
- Argonne develops the fuel cell system configuration, determines performance, identifies and sizes components, and provides this information to SA for high-volume manufacturing cost estimation
- Conducting joint life-cycle cost studies with SA

Summary: Technical Accomplishments

Validate and document the models for pressurized (S1, 2.5 atm at rated power) and low-pressure (S2, 1.5 atm at rated power) configurations

- **Stack:** Collaborated with 3M in taking cell data to validate the model for NSTFC MEA and stacks
- **Fuel Management:** Collaborated with 3M in taking data to validate the model for the anode subsystem, including impurity buildup
- **Water Management:** Analyzed the performance of planar humidifiers using Gore's sandwich membrane structure

- **Dynamic Performance**: Collaborating with 3M in taking data for building a dynamic model for stack response
- **Drive Cycle Simulations:** GCtool-Autonomie simulations for fuel economy, ownership cost, and optimum FCS operating parameters



Argonne 2012 FCS

Reference Performance Data

Stack model validation and documentation

- Collaboration with 3M to obtain reference performance data
- 50-cm^2 single cells with 3M MEAs
  - 24-μm membrane, 850 EW
  - Ternary NSTF catalyst: 0.05(a)/0.1(c) mg-Pt/cm^2 (varied)
- Data available
  - Polarization curves: Galvano dynamic scans (0.02->2->0.02 A/cm^2, 10 steps/decade, 120 s/pt, 0.1 A/cm^2 max step)
  - High frequency resistance (HFR)
  - Mass activity, ECSA, hydrogen crossover, short resistance

Series			1	2	3	4	5	6	7	8	Total	
		Variables	T	P	RH	L_{Pt}, c	SR_c	SR_a	Cold T	Idling	Tests	Status
	L_{Pt}, c	Refrence P/T										
A	0.10 mg/cm^2	1.5 atm, 80^{o}C	4	5	8	8	4	5	3	4	41	√
B	0.10 mg/cm^2	2.5 atm, 85^{o}C	4		9		4	5	3		25	√
C	0.15 mg/cm^2	1.5 atm, 80^{o}C	4	5	8		4	5	3		29	Ongoing
D	0.15 mg/cm^2	2.5 atm, 85^{o}C	4		9		4	5	3		25	Ongoing
E	0.10 mg/cm^2	2.5 atm, 85^{o}C	Effect of N_2 dilution: Variable RH, SR_a, % N_2									√
F	0.10 mg/cm^2	1.5 atm, 80^{o}C	Dynamic response to step changes in cell current density									Ongoing

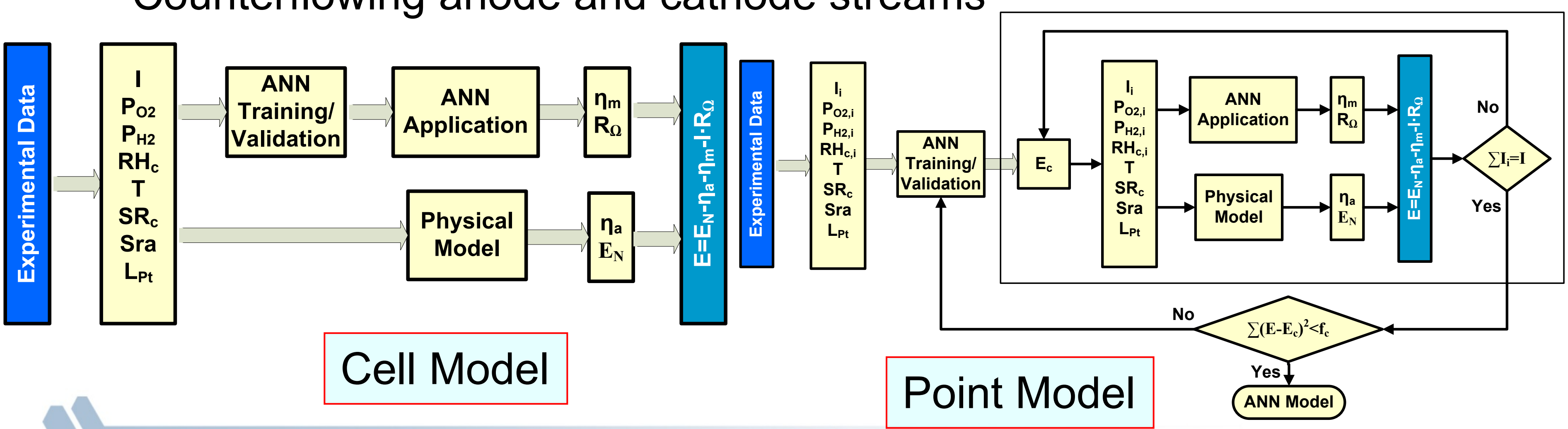
Hybrid Artificial Neural Network and Physical Model

Cell model

- Nernst equation for reversible potential
- ORR overpotential modeled as a function I, T, P_{O2} and RH_c
- Modeled HOR and anode-side mass transfer overpotentials
- Artificial Neural Network (ANN): HFR and mass transfer overpotential
- Multilayer Perceptron (MLP) Feed-Forward Network with one hidden layer and 20 neurons, hyperbolic tangent activation function

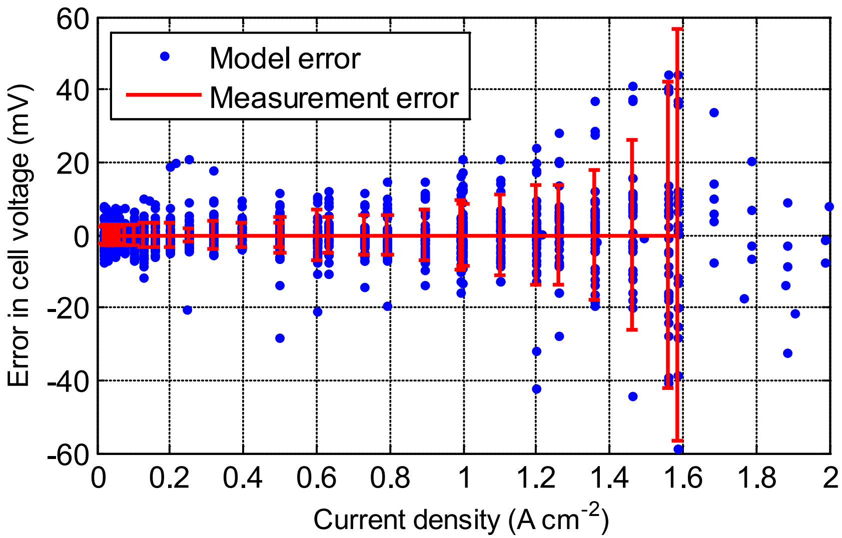
Point Model

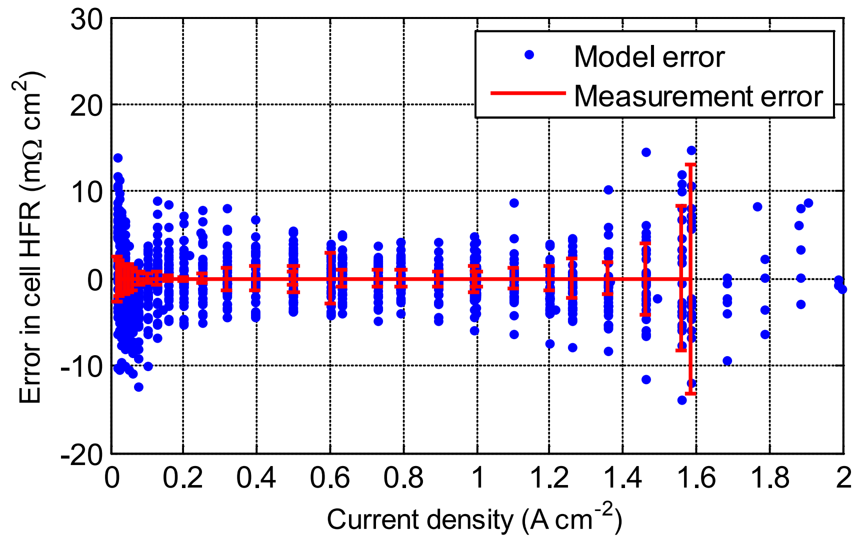
- Input vector modified for local values of I, P_{O2} and RH_c
- Counterflowing anode and cathode streams

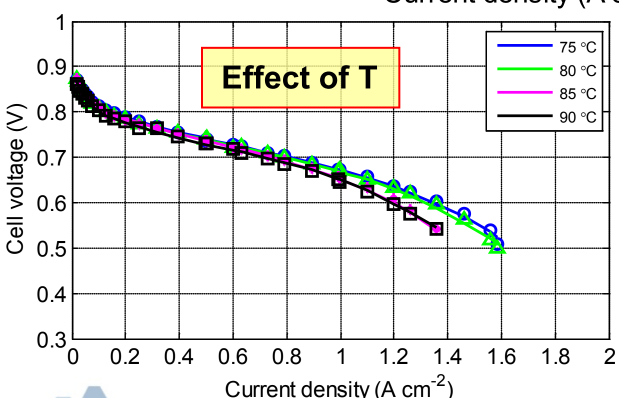


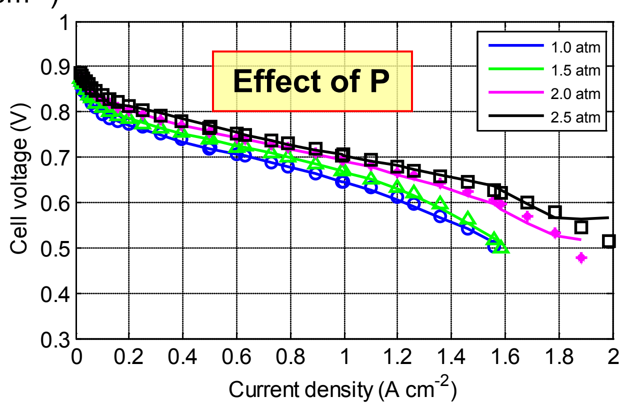
Hybrid Model Testing and Calibration

- Modeling error is comparable to variations in measured data at reference conditions (1.5 atm, 80^{o}C, 65^{o}C T_{dp}, $SR_a = SR_c = 2$, 0.1 mg/cm^2 Pt loading in cathode)
- Argonne to continue to calibrate the physics based model





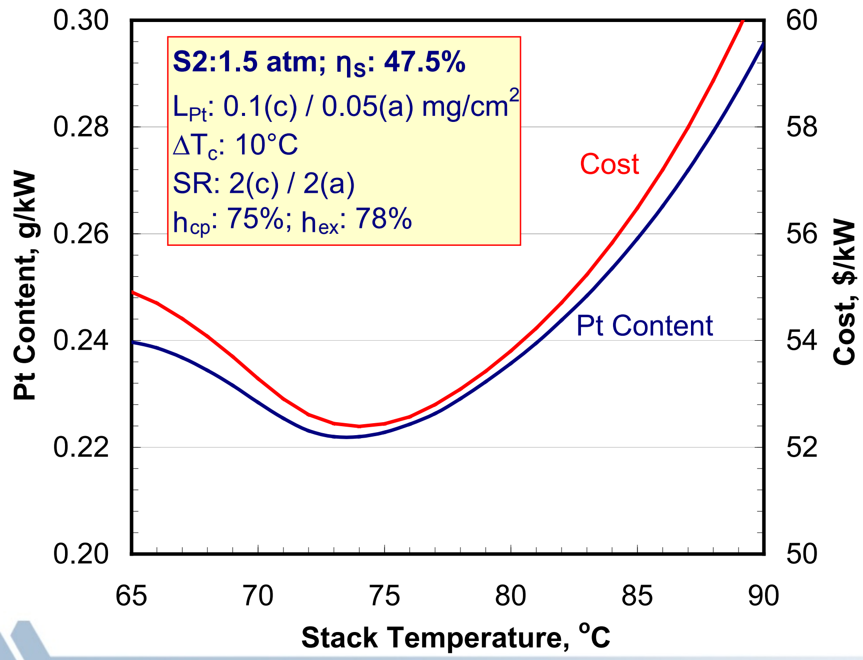


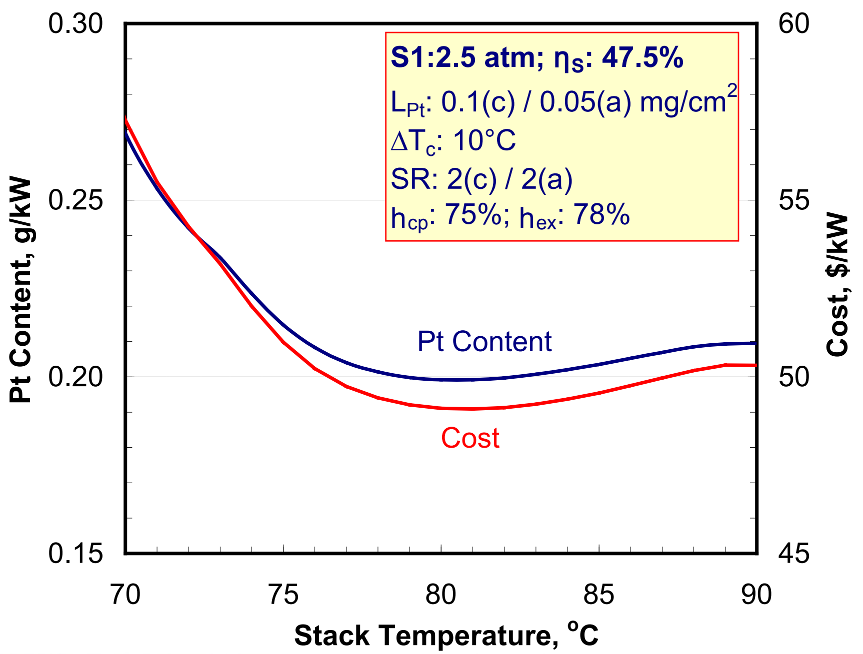


- Thresholds for minimum H_2 and air flow rates
- Isolated data points at large I not considered
- Constant P not maintained at high SR_c

Pt Content and System Cost

- Optimum stack T (same as coolant exit T) and inlet RH_c at which the Pt content and the system cost* are lowest
  - Optimum stack T depends on the operating P: 75°C at1.5-atm stack inlet P, 80°C at 2.5-atm stack inlet P
- At optimum stack T, system S1 has lower Pt content and system cost
  - 0.22 g_{Pt}/kW for system S2, 0.20 g_{Pt}//kW for system S1, η_S = 47.5%
  - $52.4/kW for system S2, $49.1/kW for system S1, η_S = 47.5%





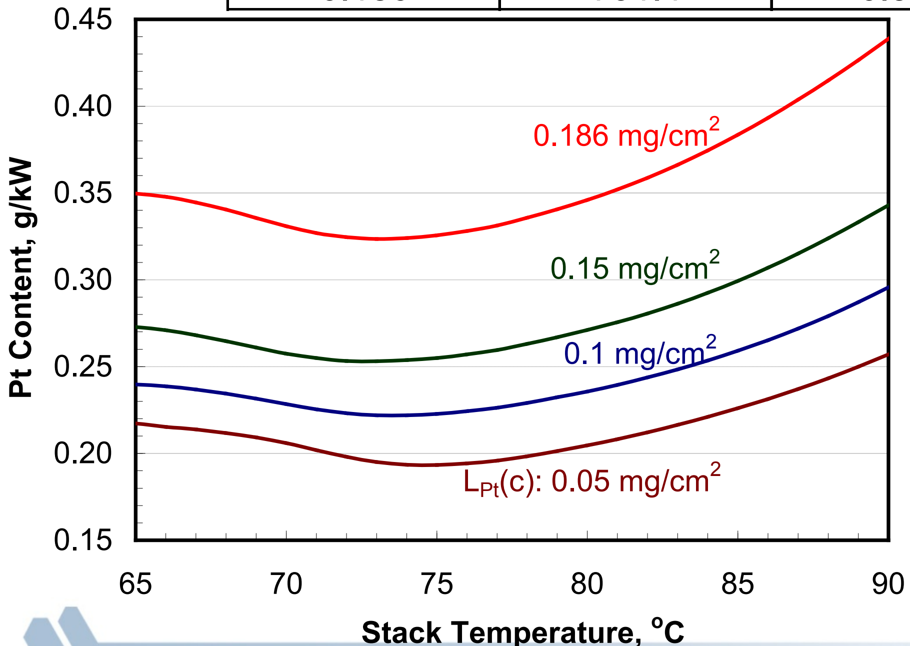
*Cost estimates from SA correlations for high volume manufacturing

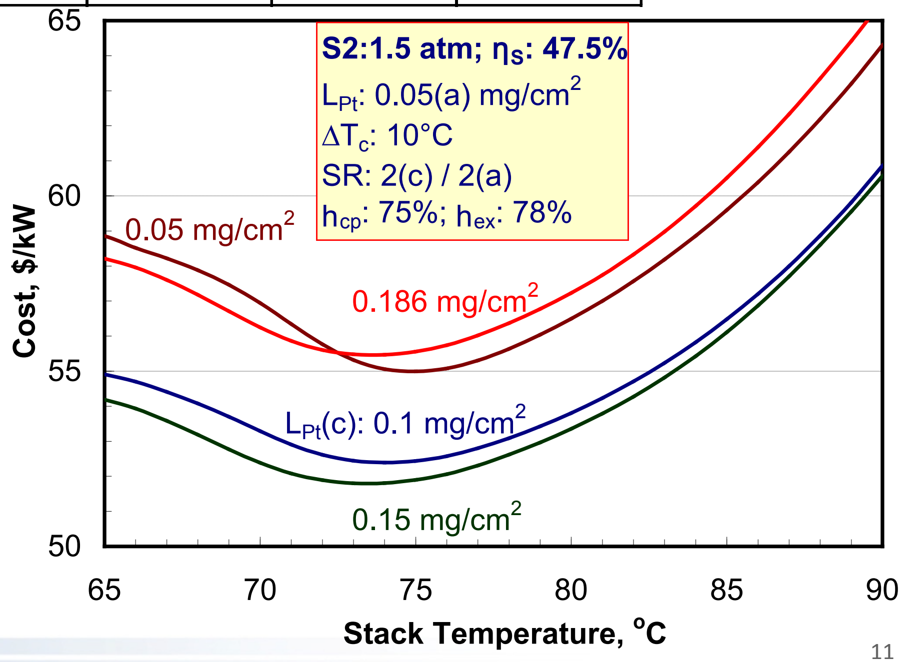
Optimum Pt Loading in NSTF Cathode Catalyst

System S2 (1.5 atm stack inlet pressure)

- Higher optimum stack T at lower Pt loading, $L_{Pt}(c)$
- Lowest Pt content with 0.05 mg/cm² Pt loading in cathode catalyst
- Lowest system cost with 0.15 mg/cm² Pt loading in cathode catalyst

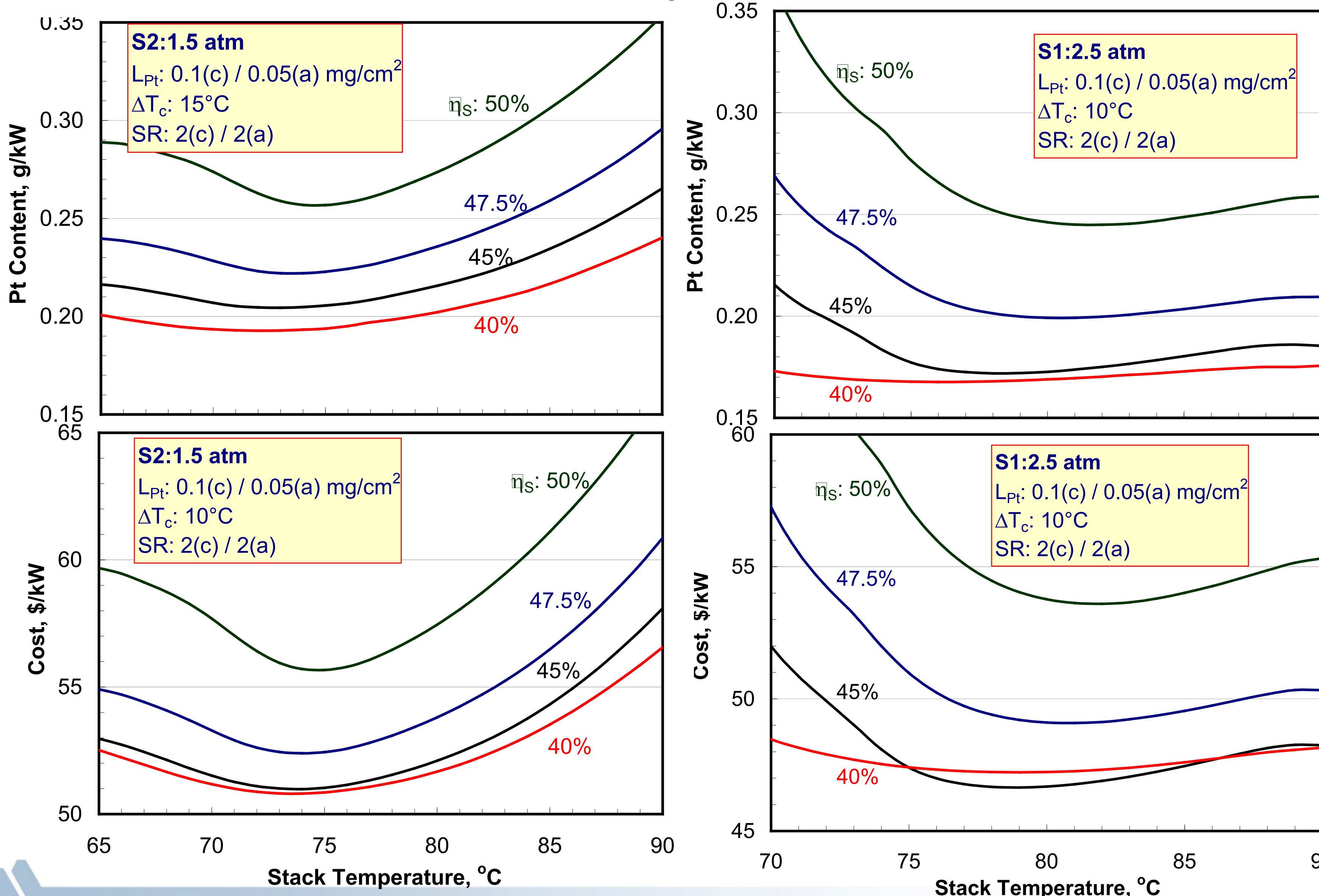
Pt Loading, c	Power Density	Pt Content	Cost ($/kW)		
mg/cm²	mW/cm²	g/kW	Pt	Stack	System
0.05	584.7	0.19	6.8	36.5	55.0
0.1	734.3	0.22	7.9	28.0	52.4
0.15	841.8	0.25	9.0	27.4	51.8
0.186	791.4	0.32	11.5	31.1	55.5





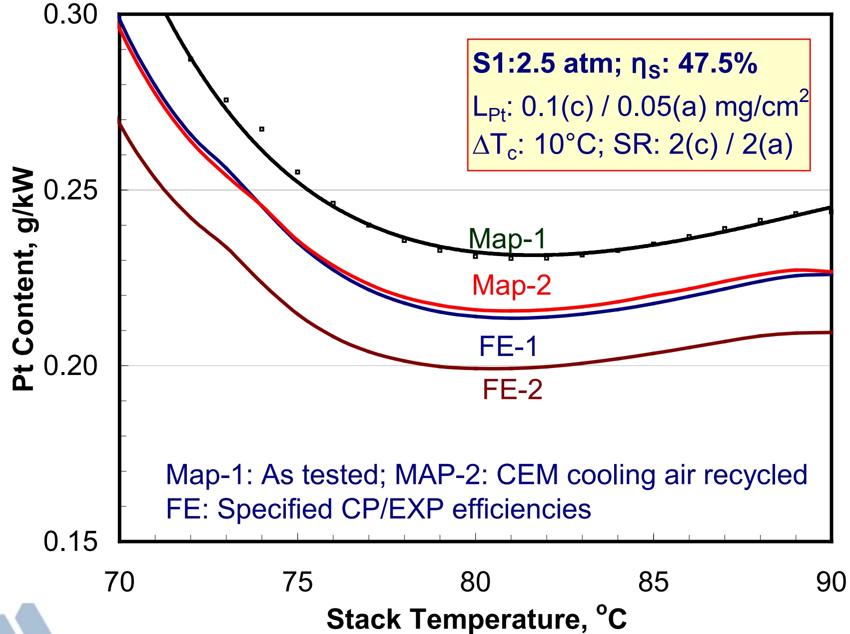
System Cost vs. System Efficiency Trade-Off

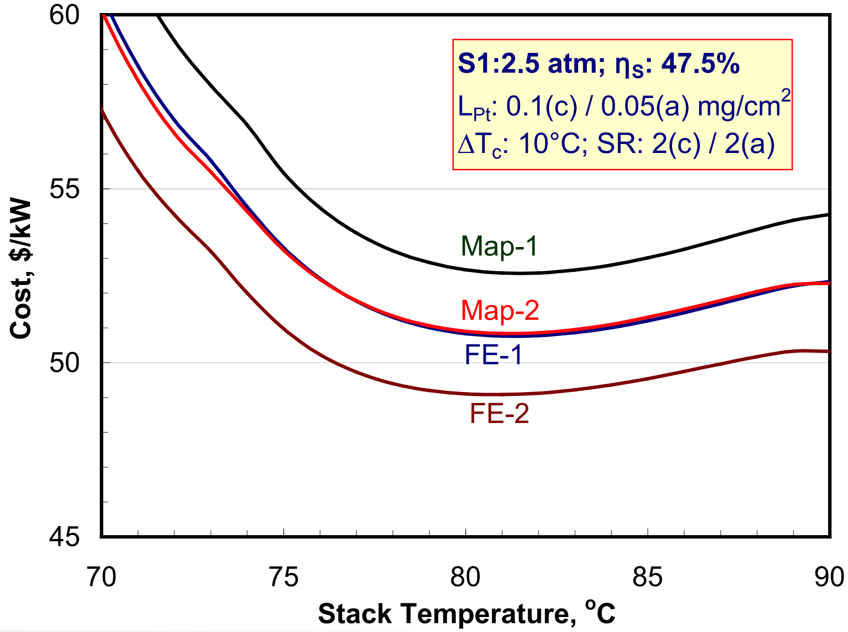
- No reduction in system cost if η_S is lowered below 40 - 45%



Air Management System

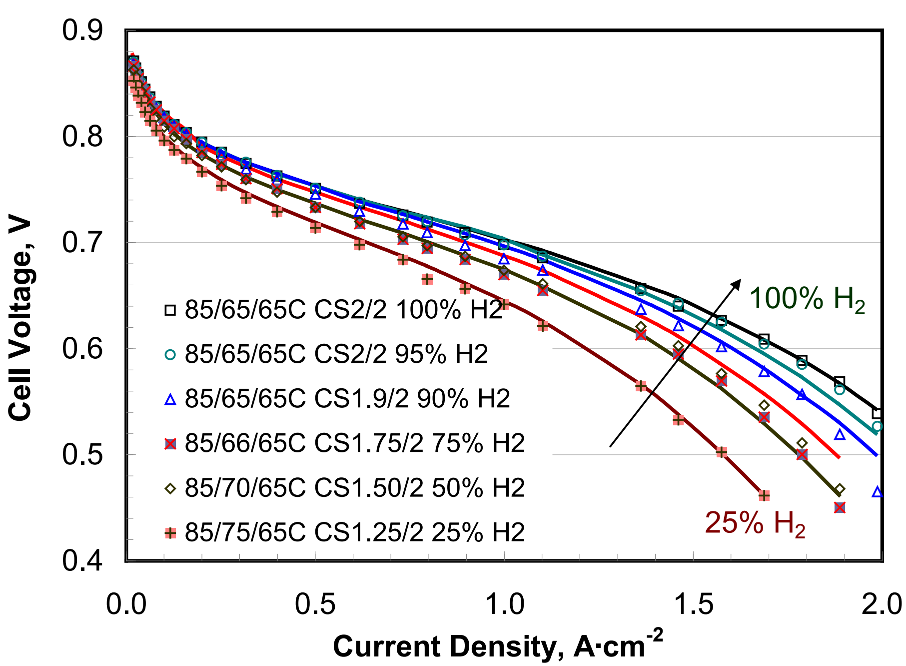
- Air Management System
  - Map-1: CEM model based on the measured performance of the components (compressor, expander, motor, controller, filter, cooling air)
  - Map-2: As in MAP-1 but bleed air that cools the motor is combined with the compressed air
  - FE-1: Same as Map-1 but fixed compressor/expander efficiencies
  - FE-2: Same as Map-2 but fixed compressor/expander efficiencies

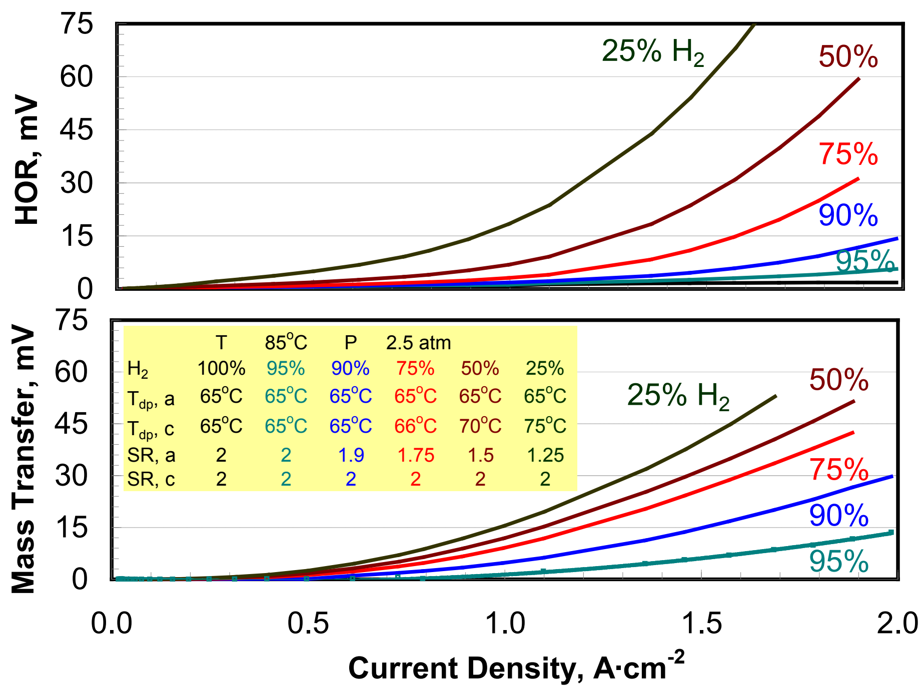




Anode Subsystem

- Collaboration with 3M to obtain data with 0-75% N_2 in H_2
  - Data at 85ºC, 2.5 atm, variable H_2 SR for constant pumping power
- Formulated anode model to determine overpotentials for HOR and mass transfer
  - Large gradients in H_2 concentration at high current densities with >10% N_2 at anode inlet

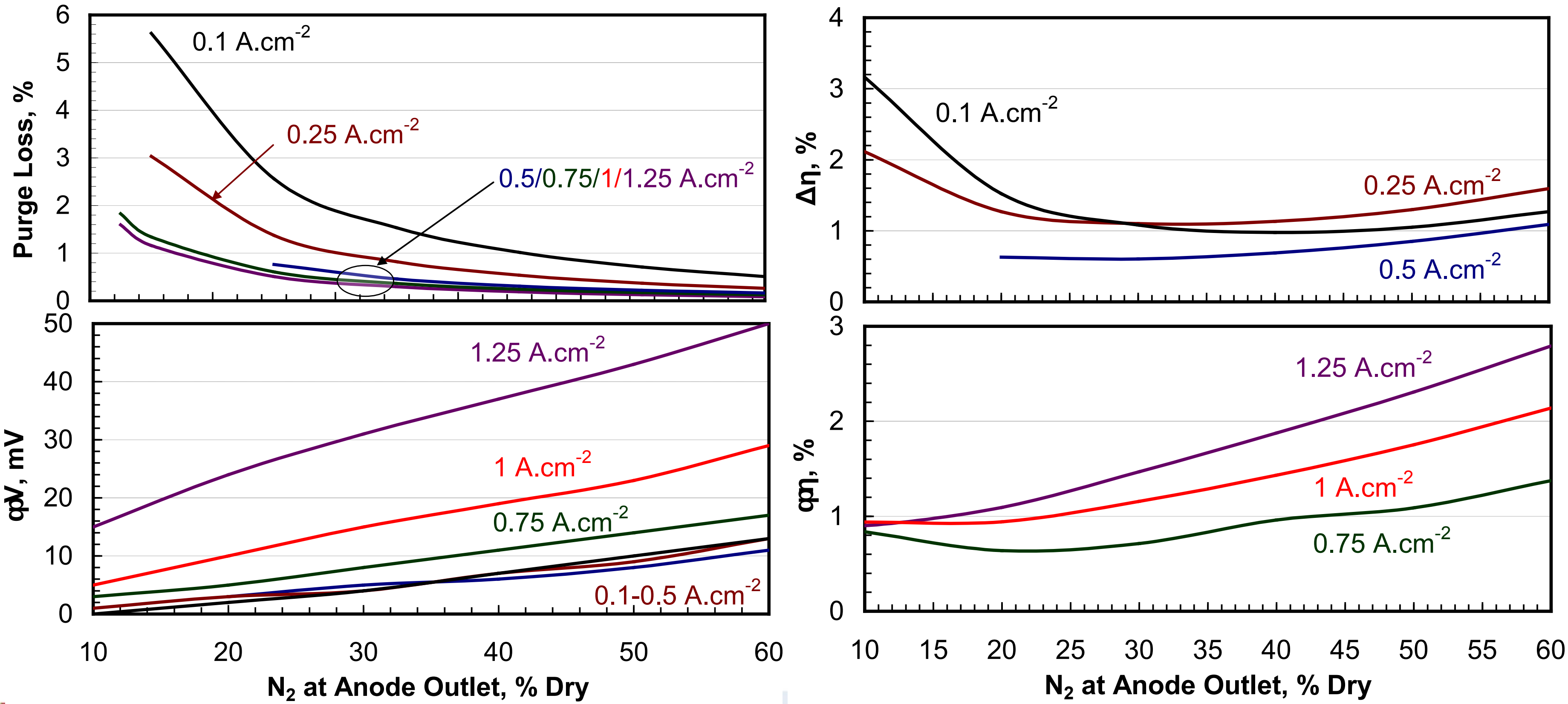




Nitrogen Buildup and Performance Losses

Dynamic simulations (system S1, variable P, 85°C); ISO H_2 quality

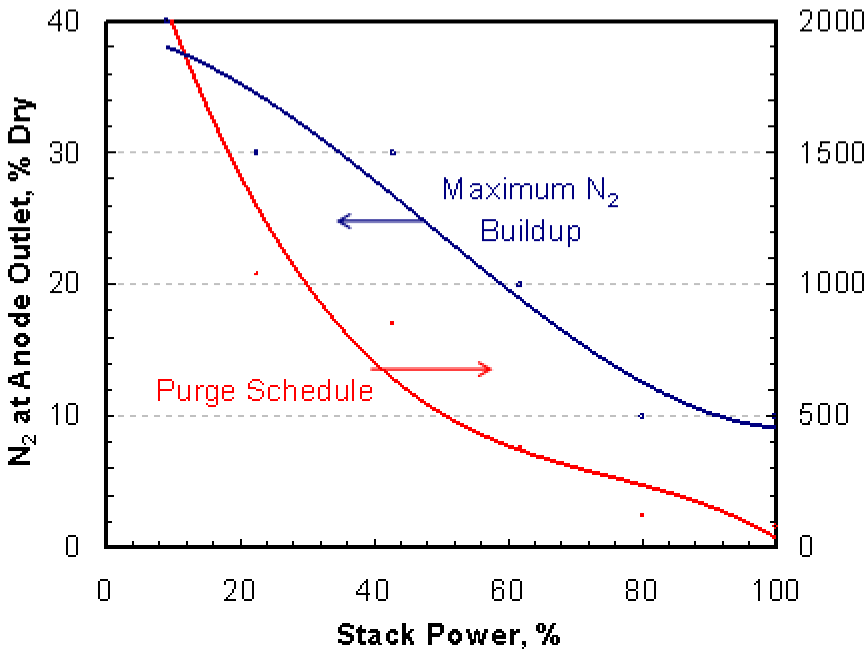
- Single purge, additional H_2 at rated flow rate, 2x anode system volume
- Smaller purge losses, but larger decrease in cell voltage, at higher power or greater allowable N_2 buildup
- For optimum efficiency, allowable N_2 buildup is a compromise between purge loss and decrease in cell voltage

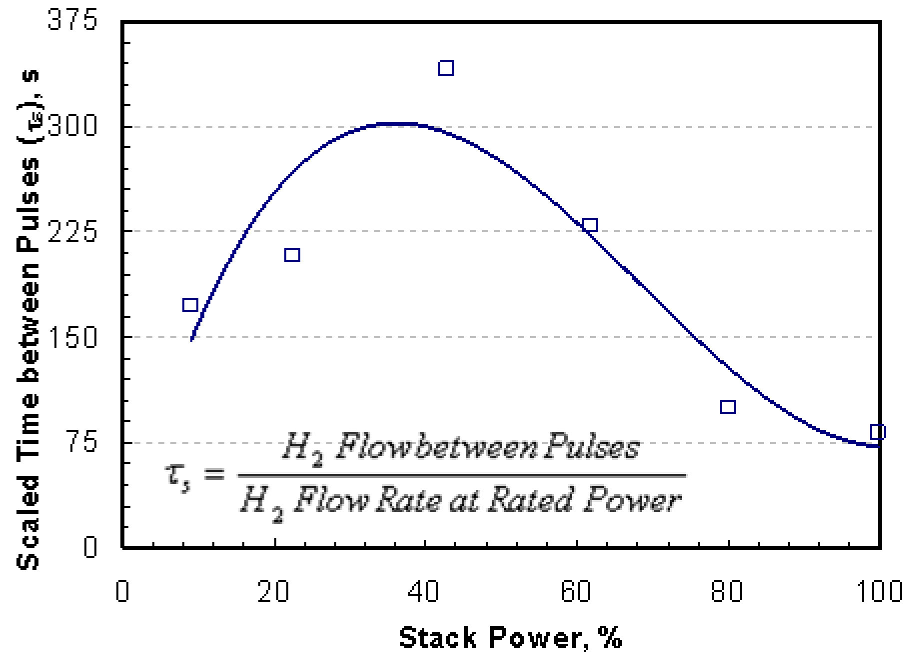


Optimum Purge Schedule

Conducted dynamic simulations at constant power to determine the optimum purge schedule and the allowable N_2 buildup

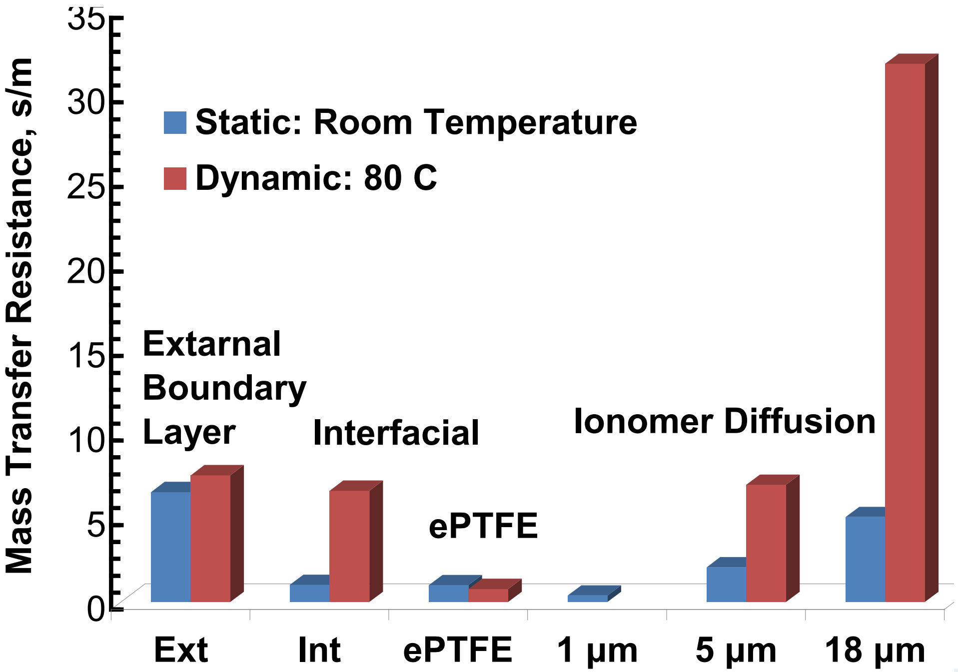
- Shorter purge schedule and smaller allowable N_2 concentration at higher power
- Developed criterion for purging anode without relying on a H_2 sensor
- Running drive-cycle simulations to verify and improve dynamic optimum purge criterion

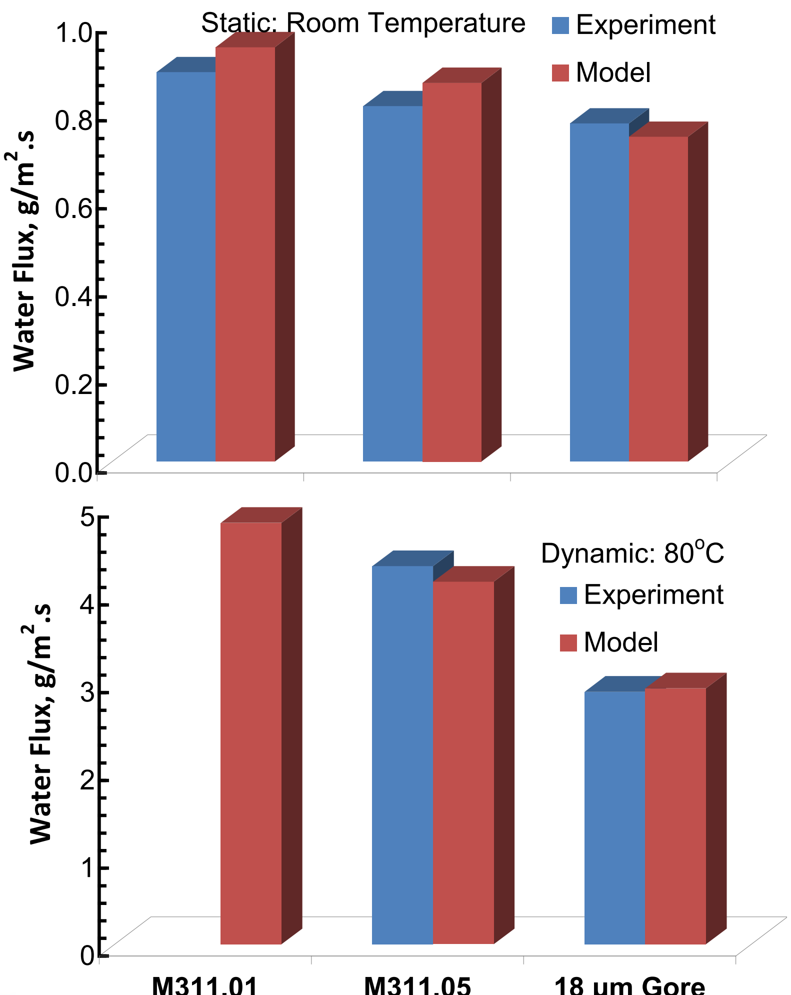




Water Management Subsystem

- Extended the membrane humidifier model to Gore's sandwich structure (W. B. Johnson, FC067)
  - Determined mass transfer resistances; external boundary layer, interfacial, ePTFE, and ionomer
  - $R = 2R_{ext} + 2R_{int} + 2R_{PTFE} + R_{ion}$
  - Validated model against static and dynamic data

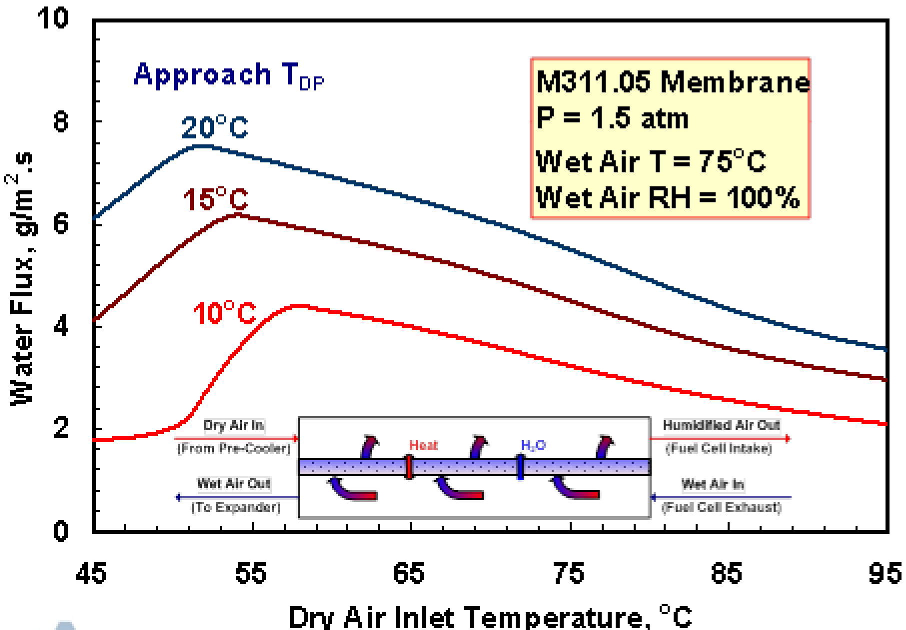


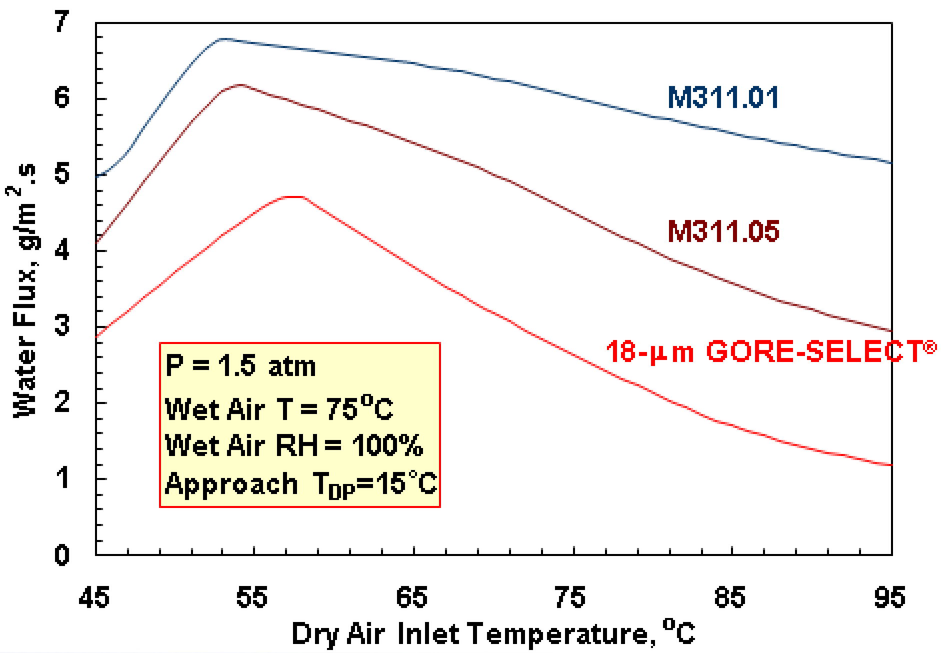


Humidifier Performance

Determined dry air inlet temperature for maximum water transfer flux, planar counter-flow humidifier

- Air pre-cooler needed, optimum amount of pre-cooling (T_m) is a function of approach dew-point temperature, T_{dp}(wet-in) - T_{dp}(dry-out)
  - Flux may be limited by saturation condition for $T < T_m$, by diffusivity in ionomer for $T > T_m$
- Compared to 18-μm GORE-SELECT® membrane, water flux can be 30% higher in M311.05 and 45% higher in M311.01

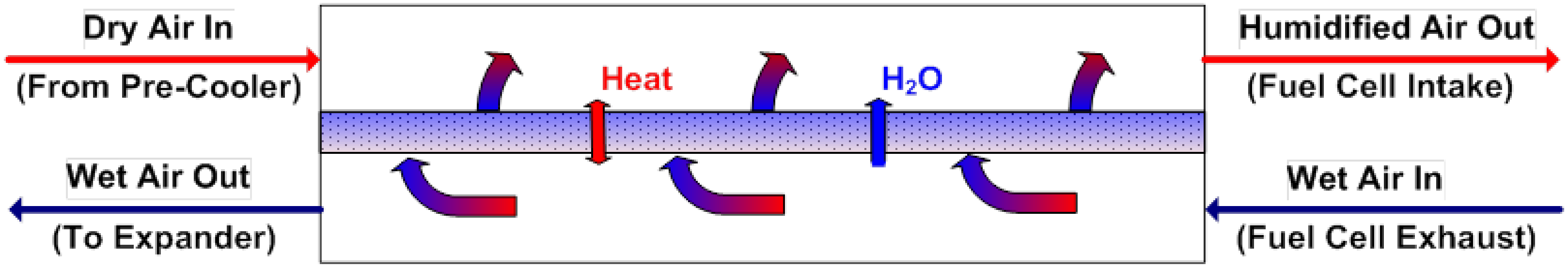


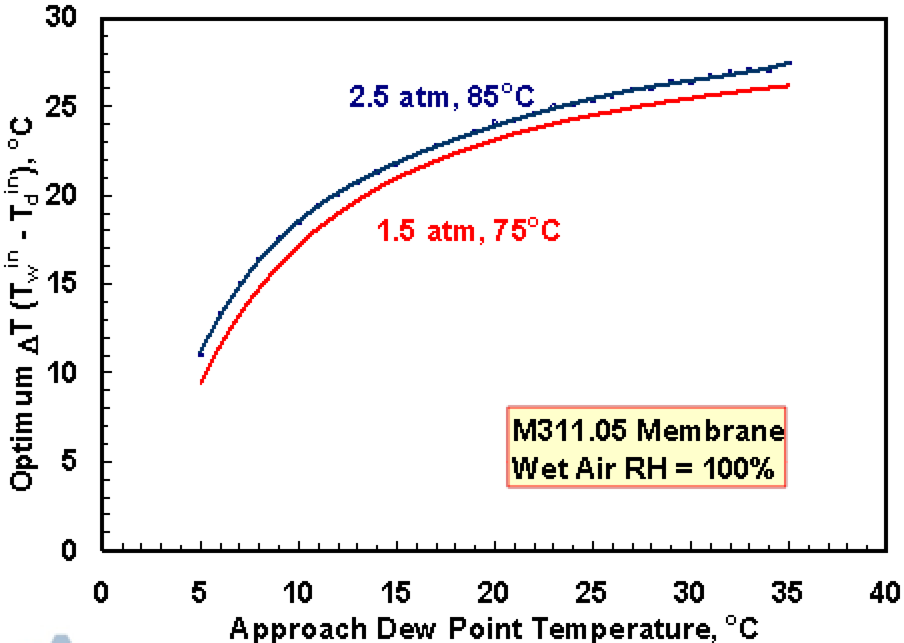


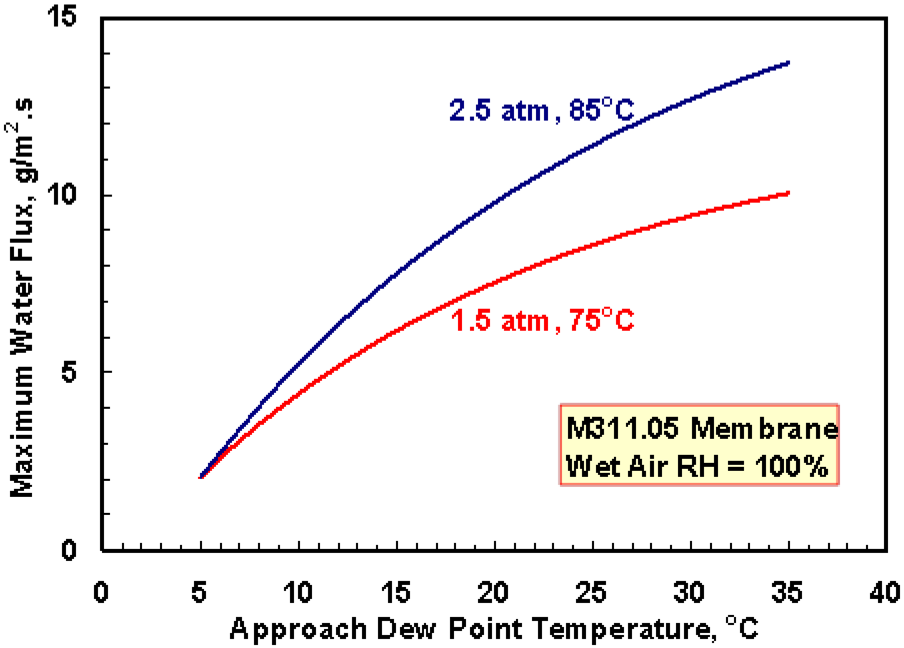
Optimized Humidifier Performance

The humidifier in S1 (2.5 atm) system can be more compact than in S2

- Higher water flux, smaller required water transfer rate



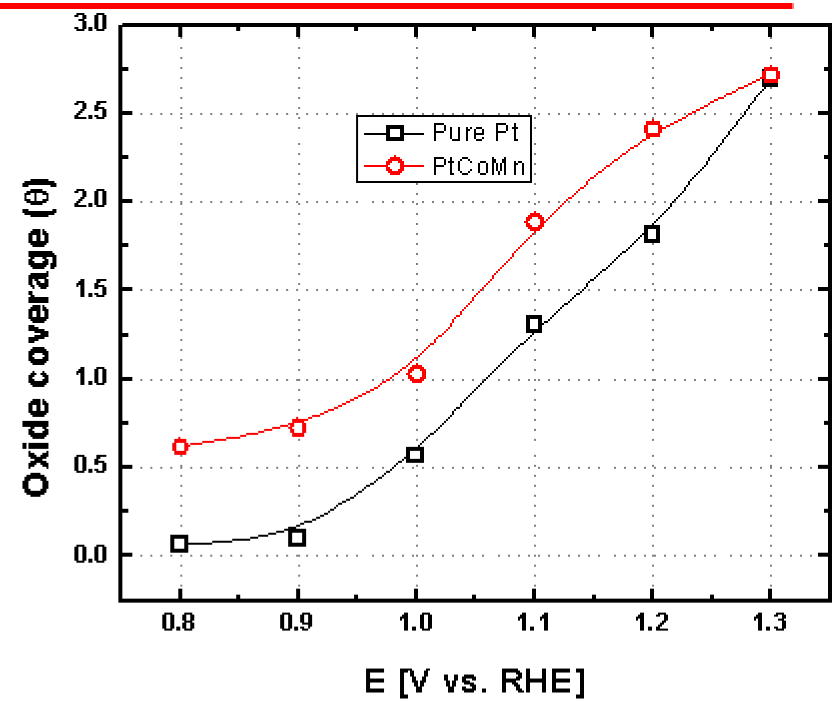


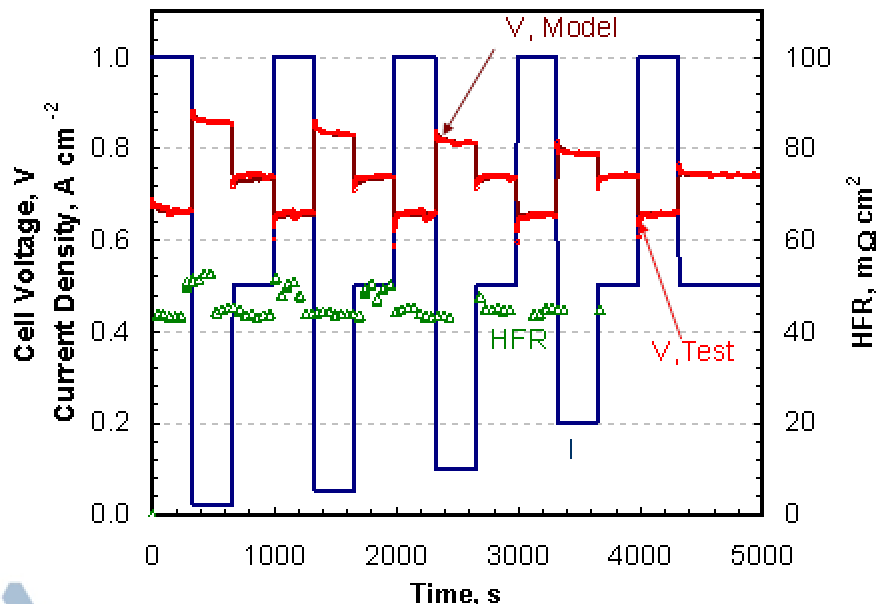


Concurrent Activity: Dynamic Performance

Dynamics of oxide growth

- Measured oxide coverage on 3M pure Pt and ternary catalysts on whiskers after 8-h holds at CV potentials
- Analyzing dynamics of oxide growth using equilibrium coverages and CV scans





Dynamics of mass transfer

- Working with 3M to measure voltage response to step changes in current density
- Modeling transient polarization data during up-scans and down-scans

Future Work

- Support DOE/U.S. DRIVE development effort at system, component, and phenomenological levels
- Continue collaboration with 3M to validate, calibrate and document the stack model
  - Alternate membranes, catalyst structures, and system configurations
- Continue cooperation with partners to validate air, fuel, thermal, and water management models
  - Establish closer collaborations with the OEMs
- Support SA in high-volume manufacturing cost projections, collaborate in life-cycle cost studies
- Collaborate with 3M to develop durability models for NSTFC electrode structures
  - System optimization for cost, performance, and durability
  - Drive cycle simulations for durability enhancement
- GCtool model of PEFC systems for fork-lift applications and CHP

Project Summary

Relevance:	Independent analysis to assess design-point, part-load and dynamic performance of automotive and stationary FCS
Approach:	Develop and validate versatile system design and analysis tools Apply models to issues of current interest Collaborate with other organizations to obtain data and apply models
Progress:	Determined the operating conditions for reducing the PGM content to less than 0.2 g/kW and FCS cost to less than \$50/kW Validated the earlier conclusion that S1 (2.5-atm) is a lower cost option than S2 (1.5 atm) in spite of the higher parasitic power Demonstrated that 0.1-0.15 mg/cm^2 Pt loading in NSTF cathode leads to lowest system cost Developed criteria for purging anode to limit H_2 loss and cell voltage degradation Showed that water flux in a planar humidifier can be enhanced by 30-45% with Gore's M311.05 and M311.01 membranes
Collaborations:	3M, Gore, SA, ANL (Autonomie)
Future Work:	Finish on-going analysis of 0.15 mg-Pt/cm^2 data Continue 3M collaboration for analyzing dynamic response Develop dynamic criteria for purging anodes

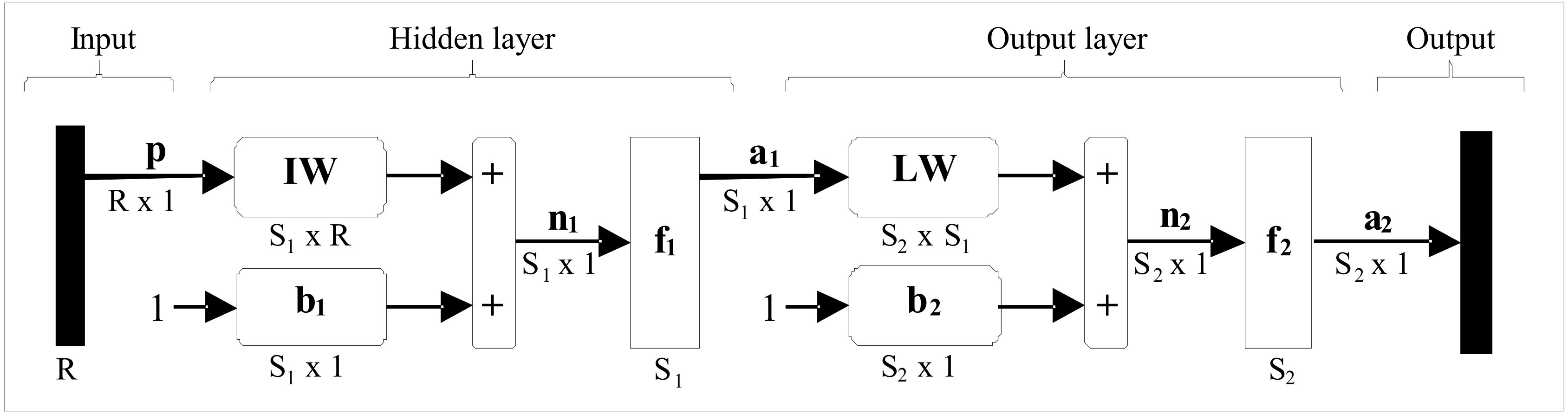
Technical Backup Slides

Artificial Neural Network (ANN)

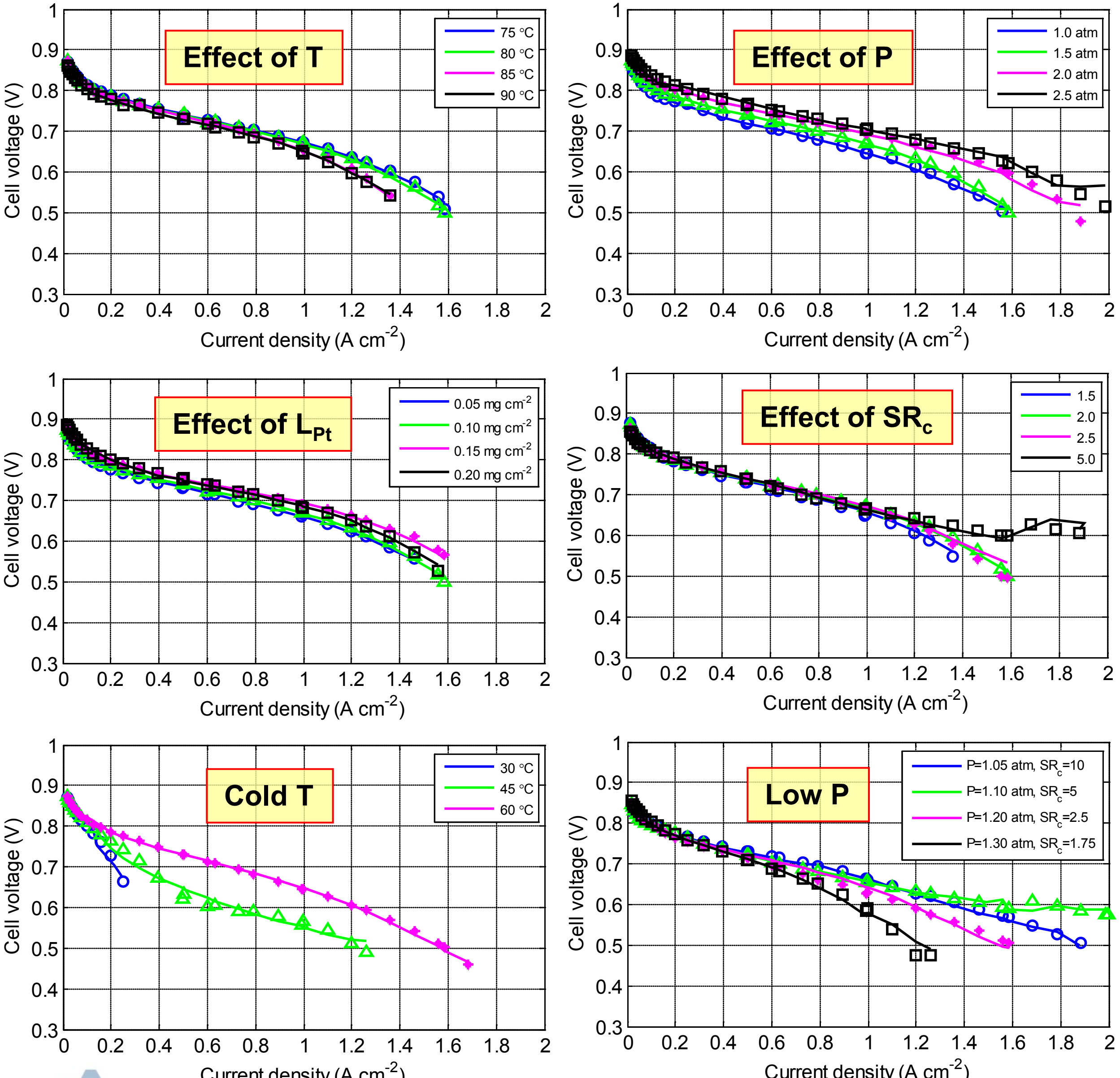
- Multilayer Perceptron (MLP) Feed-Forward Network
- One hidden layer with 20 neurons
- Output layer with 2 neurons
- Activation function: hyperbolic tangent
- Transfer function: linear

$$E = \sum LW \tanh\left(\sum IW\vec{p} + b_1\right) + b_2$$

$$\vec{p} = [P_{H_2}, P_{O_2}, RH_c, I, T, L_{Pt}, SR_c, SR_a]$$



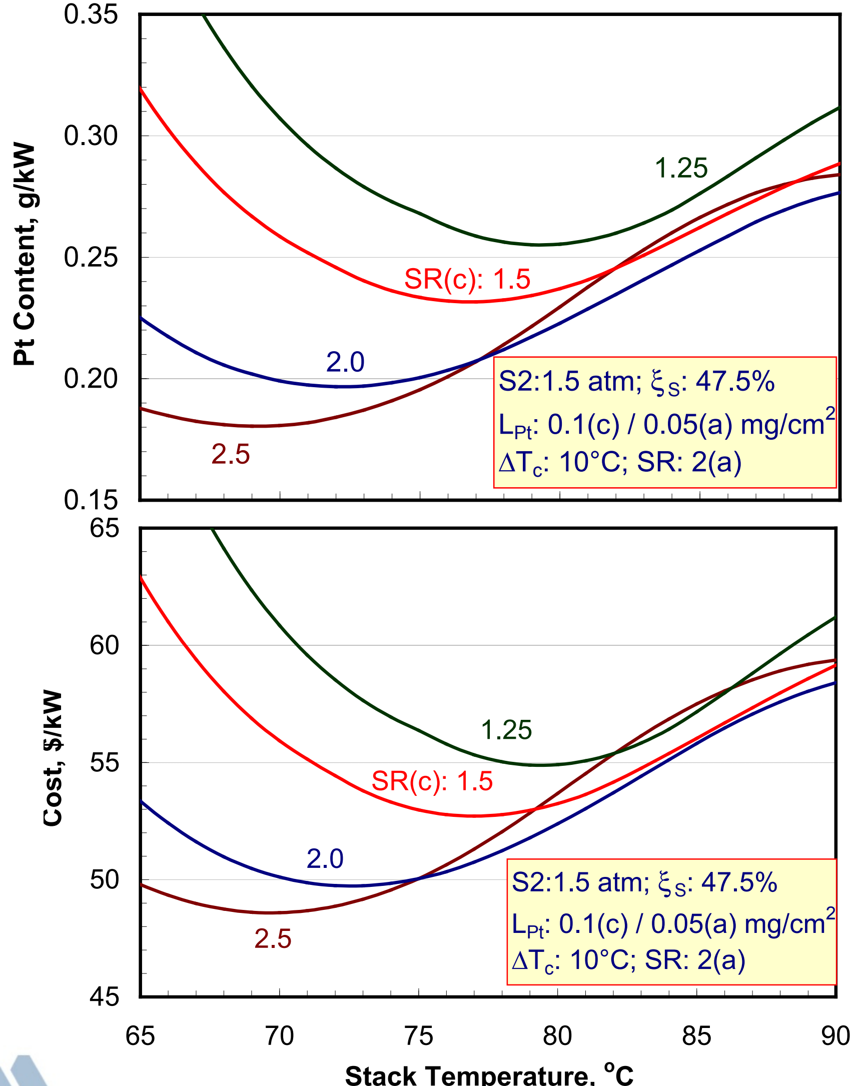
Model Testing and Calibration

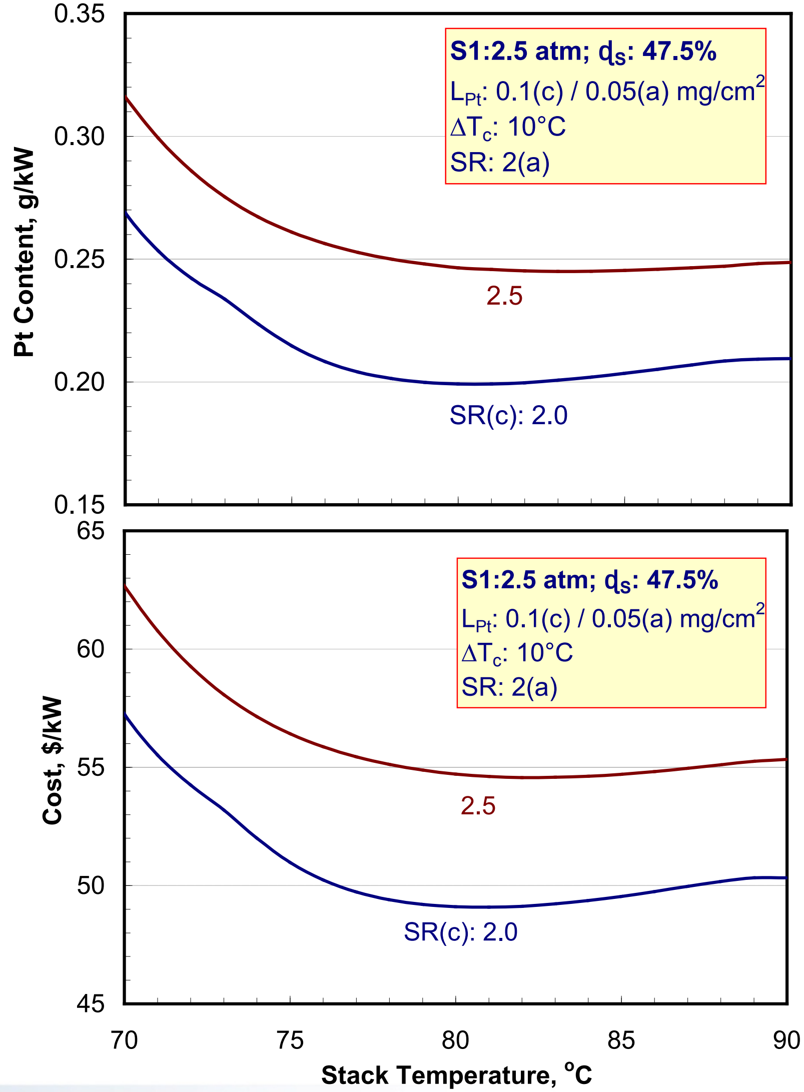


- Thresholds for minimum H_2 and air flow rates
- Isolated data points at large I not considered
- Constant P not maintained at high SR_c

Air Management System: Oxygen Stoichiometry

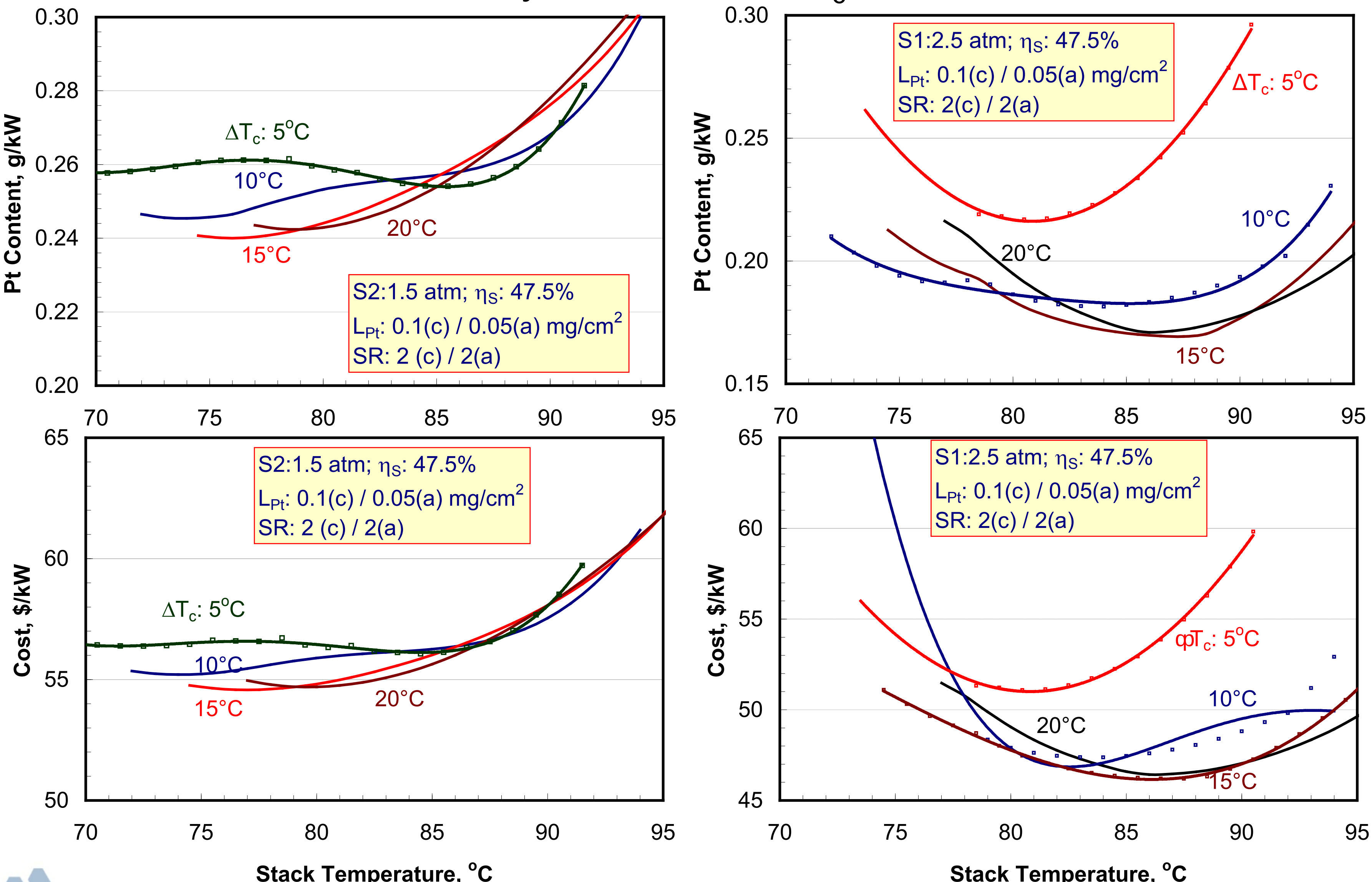
Pt content and system cost lower are lower at SR(c) < 2 for system S1 and at SR(c) > 2 for system S2





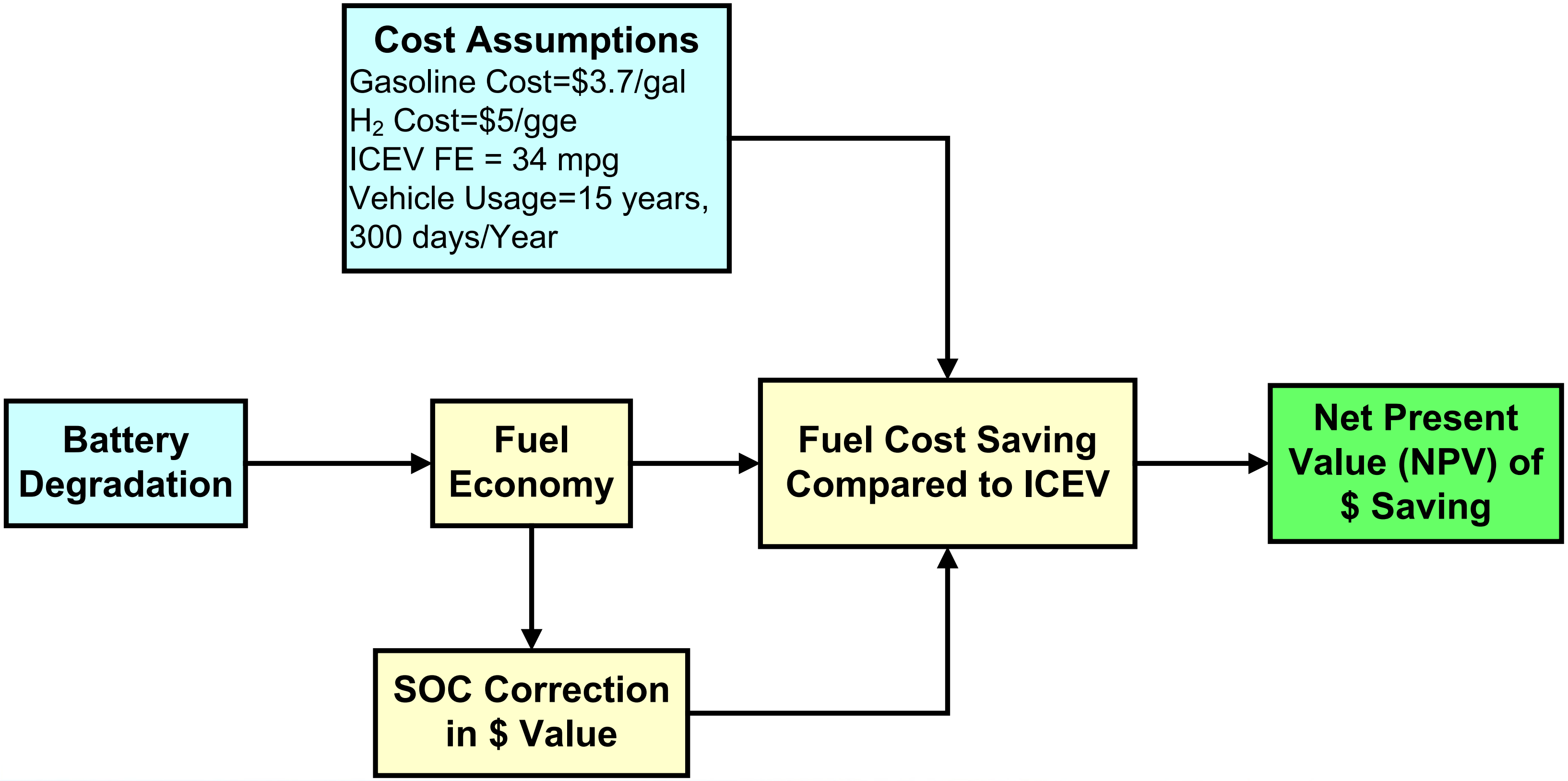
Sensitivity Study: Coolant Temperature Rise

- Lowest Pt content and system cost for ΔT_c = 15 – 20°C



Net Present Value (NPV)

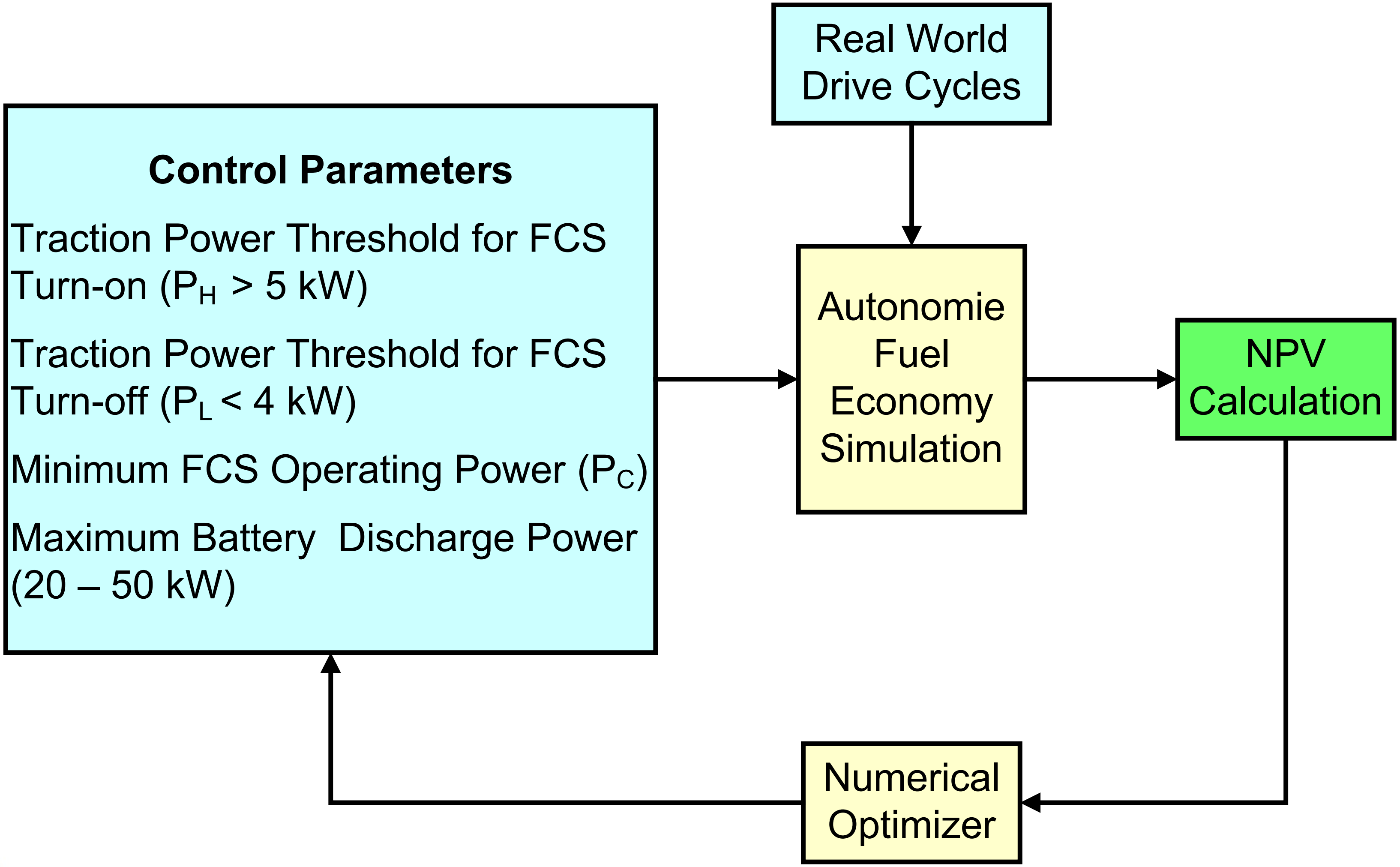
- Vehicle usage drive pattern over 15 years: 240,000 km
  - 0.7 factor applied to fuel economy of ICEV and FC HEV
- No battery or FCS replacement, no recycling cost
  - 4%/year degradation in battery performance after first 6 years
- Policy neutral study: tax incentives, fuel taxes, interest on initial cost not considered



NPV Optimization Algorithm

NPV maximized by varying battery power and FCS control parameters

- Direct search numerical optimizer, parallel computing workstations



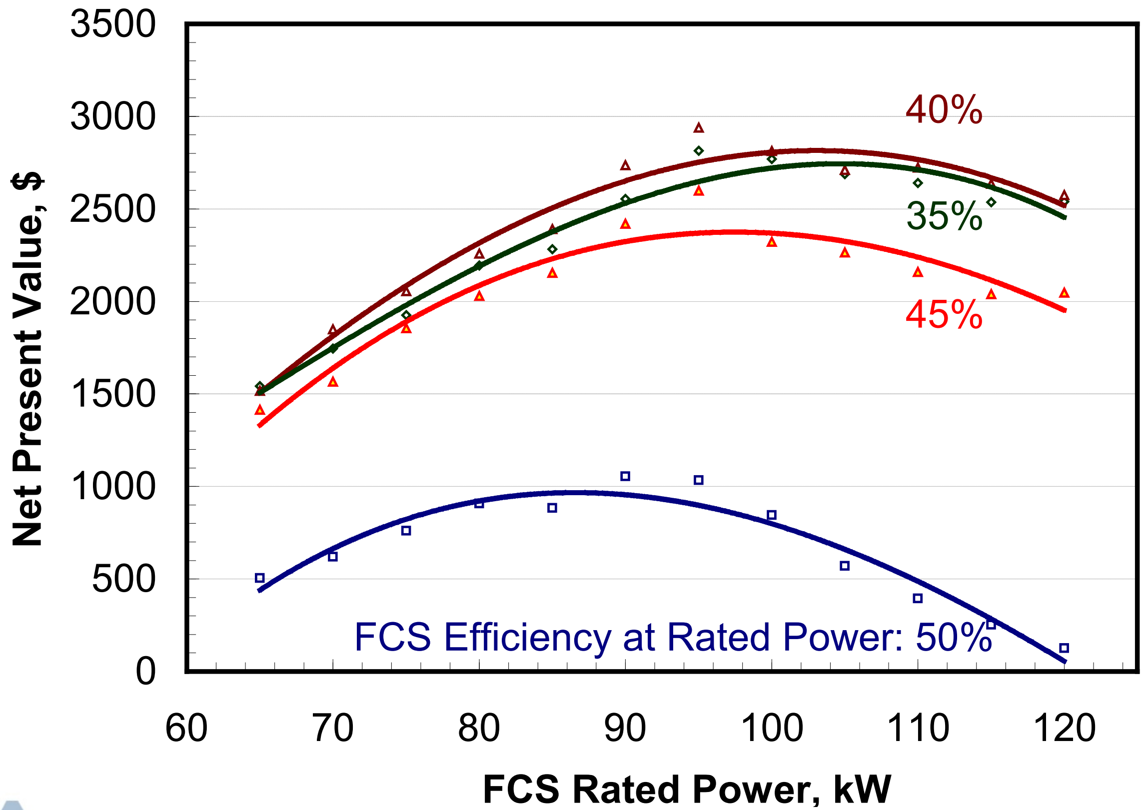
Optimum FCS Rated Power (P_R) and Efficiency (η_R)

Relationship between optimum η_R and P_R

- Optimum P_R lower for systems with higher η_R

Highest NPV for 100-kW FCS with 40% efficiency at rated power

- NPV smaller for 35% efficiency system due to higher fuel cost
- NPV smaller for 45-50% efficiency systems due to higher initial cost

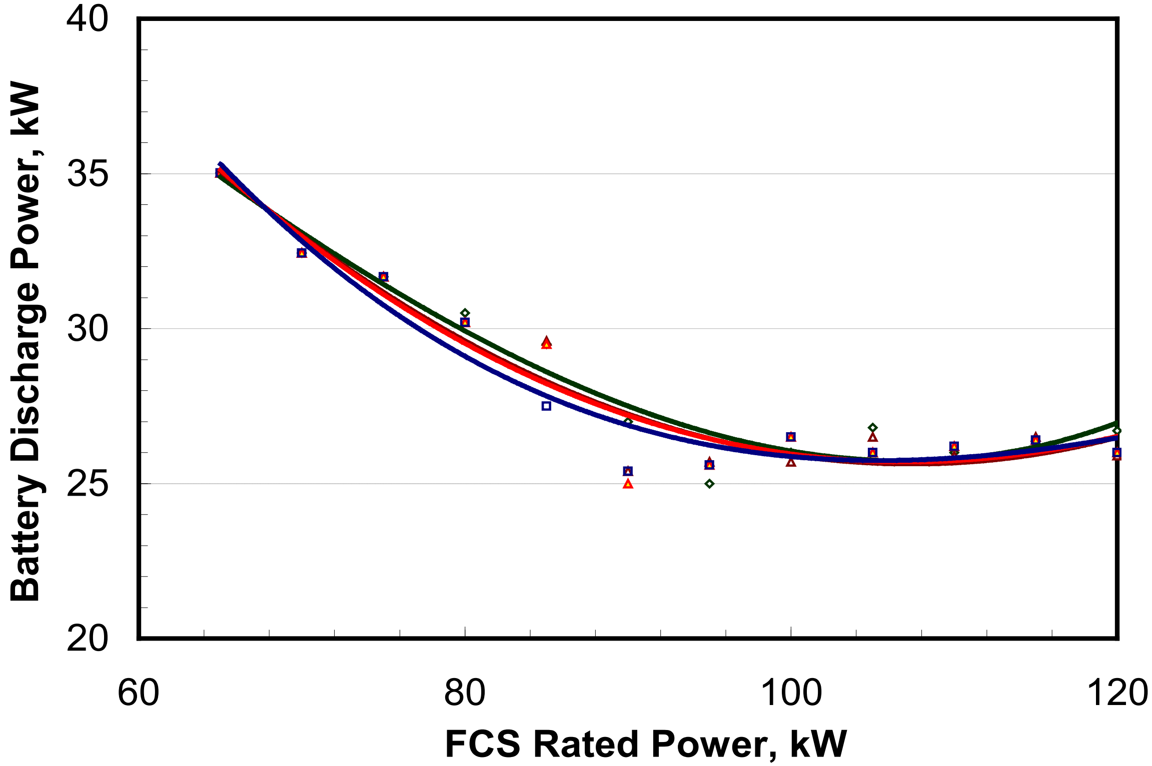


Reference Conditions
Gasoline cost: \$3.70 gal^{-1}
H_2 cost: \$5.00 gge^{-1}
ICEV adjusted FE: 23.8 mpg

Optimum Battery Discharge Power

Optimum battery discharge power generally decreases with increase in FCS power

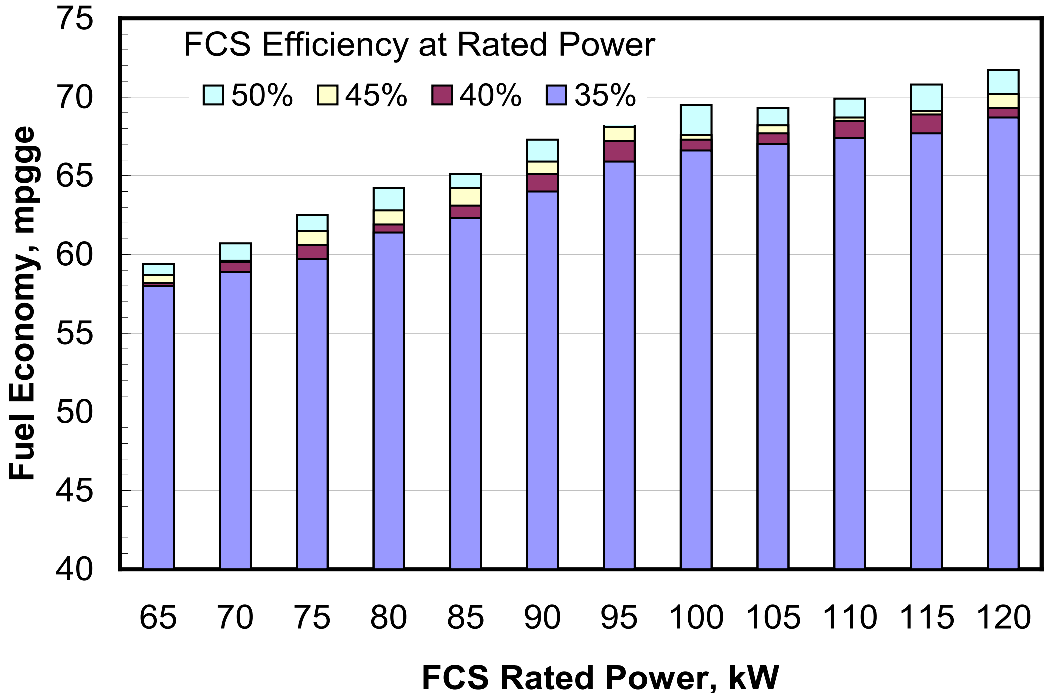
- Weak dependence on FCS efficiency at rated power
- Regenerative braking energy function of discharge power
- Acceleration depends on combined FCS and ESS power



Fuel Economy

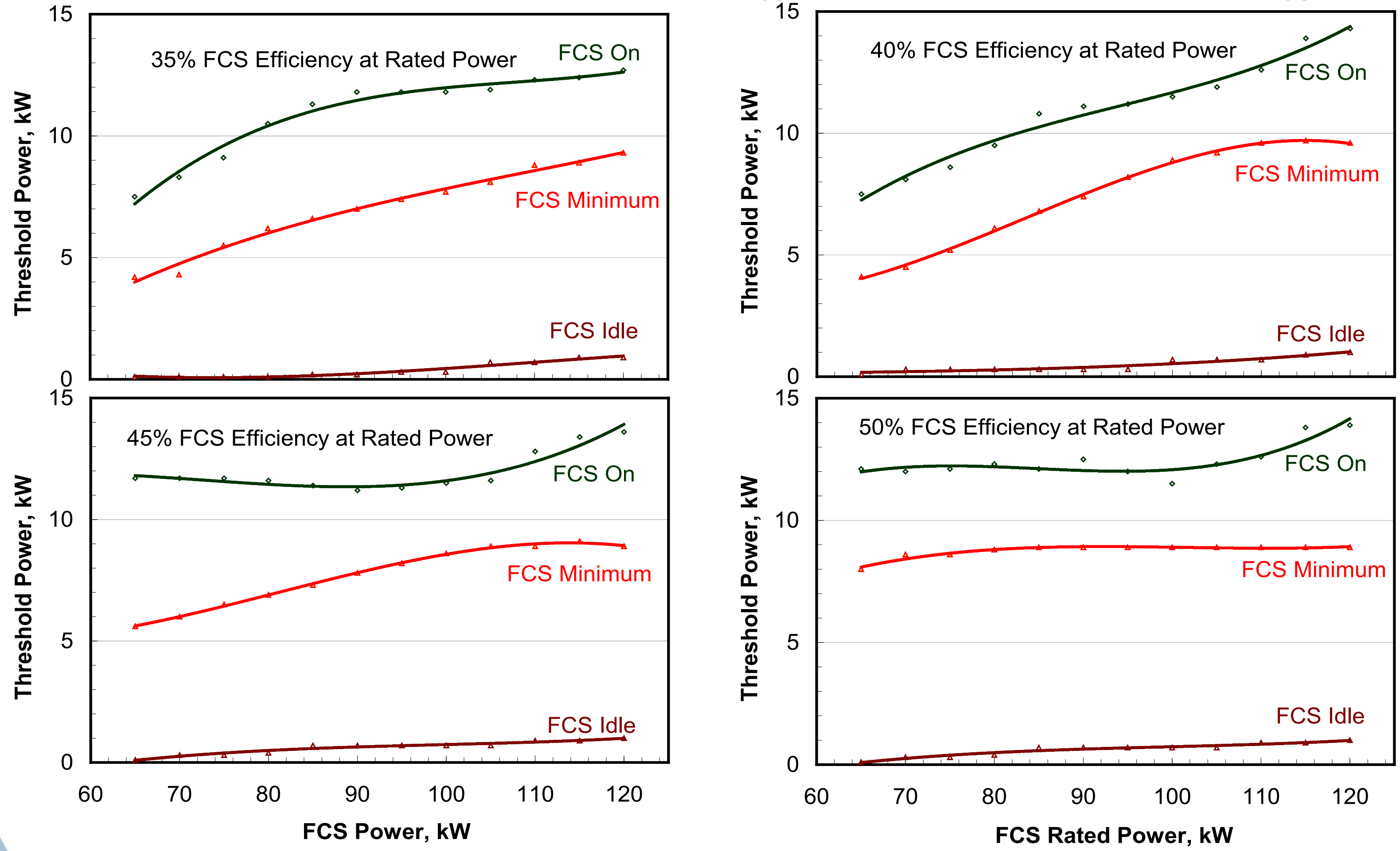
Average fuel economy over the 30 RW drive cycles and 15 years

- 0.7 factor applied to calculated FE to account for other accessory loads and ambient conditions
- Higher fuel economy for vehicles with larger FCS rated power (P_R)
- Fuel economy only weekly dependent on FCS efficiency at rated power (η_R)



Optimum FCS Control Parameters

- Proper energy management strategy allows FCS to operate down to low traction loads (P_L)
- Minimum FCS power (P_C) close to but < FCS peak efficiency point (P_m)
- Optimum traction power for FCS (P_H) turn-on is function of P_R and η_R



Optimum control strategy will also depend on stack/battery durability considerations

Sensitivity to Fuel Cost

- NPVs turn negative as H_2 cost increases to \$7.00 gge^{-1}
- No change in NPV trend over \$3.50-7.00 gge^{-1} H_2 cost - max NPV at 40% η_R
- Nearly 15 kW increase in optimum P_R with \$3.50 gge^{-1} increase in H_2 cost