Prediction of Corrosion of Advanced Materials and Fabricated Components

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Summary

- **Goal:** Develop a software tool for predicting localized corrosion of process equipment including fabricated components as well as base alloys
- **Challenge:** There is no generally accepted basis for judging the corrosion performance of materials in process environments without performing specific tests. Recently developed prediction methods need to be parameterized for complex environments and extended to fabricated materials.
- **Benefits:** Allow process designers and operators to evaluate materials in realistically modeled chemical environments, identify process changes, inhibition strategies; energy savings of 8.8e13 Btu/year
- **Potential End-User Applications:** In chemical process industries, designing/optimizing/revamping processes to eliminate/reduce aqueous corrosion problems; predicting useful life of existing equipment
- **FY05 activities:** Development of microchemistry database and electrochemical parameter database, parameterization of models, relating electrochemical parameters to alloy composition

Participants:

- OLI Systems
- Southwest Research Institute
- Haynes International
- Bechtel-Bettis
- ChevronTexaco
- DuPont
- Shell
- Mitsubishi Chemical
- Toyo Engineering

Barrier - Pathway Approach

Barriers

- Lack of tools to evaluate performance of metals prior to placing them in service

Pathways:

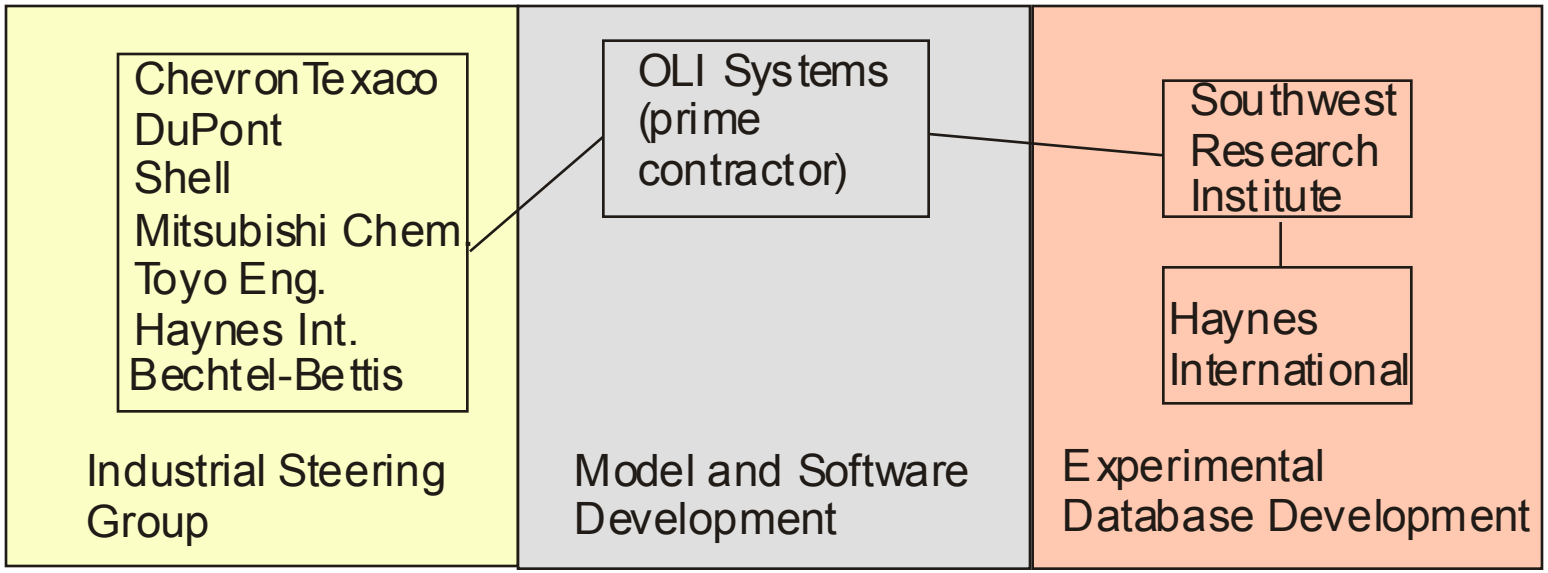
- Quantitatively relate localized corrosion parameters to solution chemistry based on sound theory
- Relate local composition of alloys with parameters that govern localized corrosion (corrosion and repassivation potentials)
- Develop a model for predicting remaining life based on short-term data
- Encapsulate the model in software – a virtual testing laboratory

Metrics:

- Quantitatively validate the accuracy of prediction of corrosion and repassivation potentials as functions of environment
- Quantitatively verify the agreement of the model with standard tests for base alloys and fabricated materials
- Verify the validity of methods for predicting remaining life

Energy savings	8.8e13 Btu/year
Cost savings - design	$400 million
Cost savings-operations	$300 - $600 million
Carbon reduction	0.87 MMTCe

Project Team



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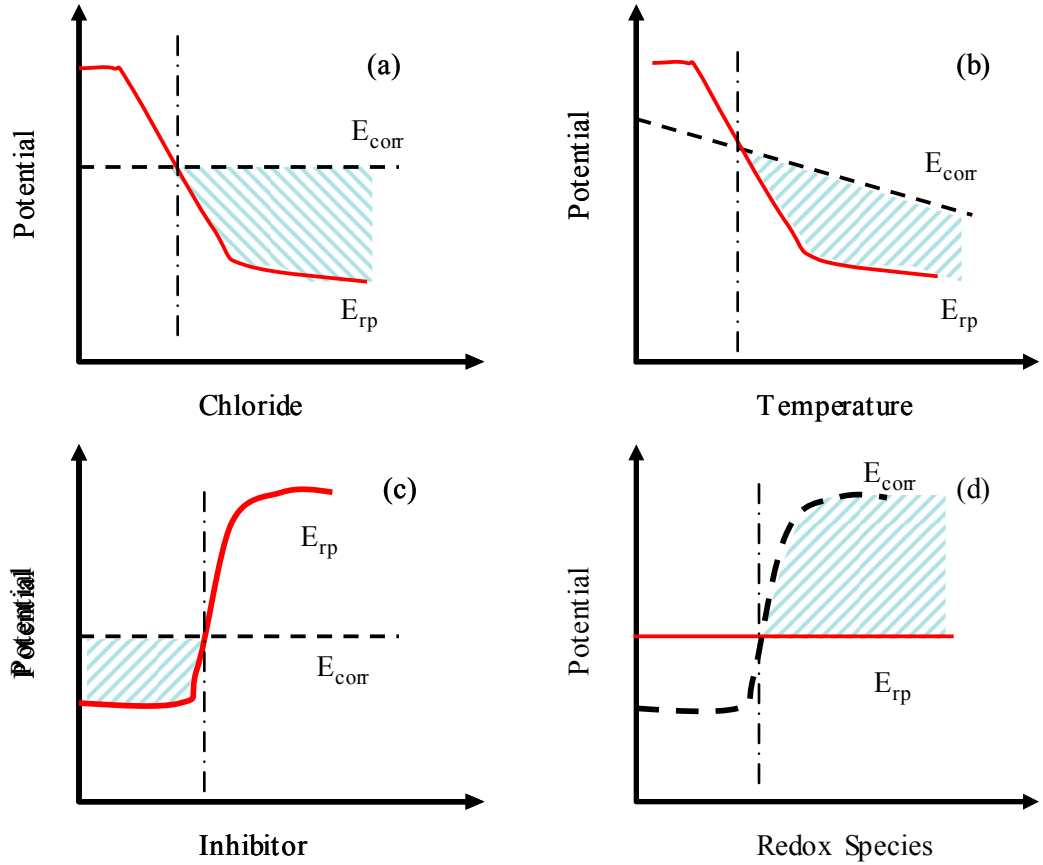
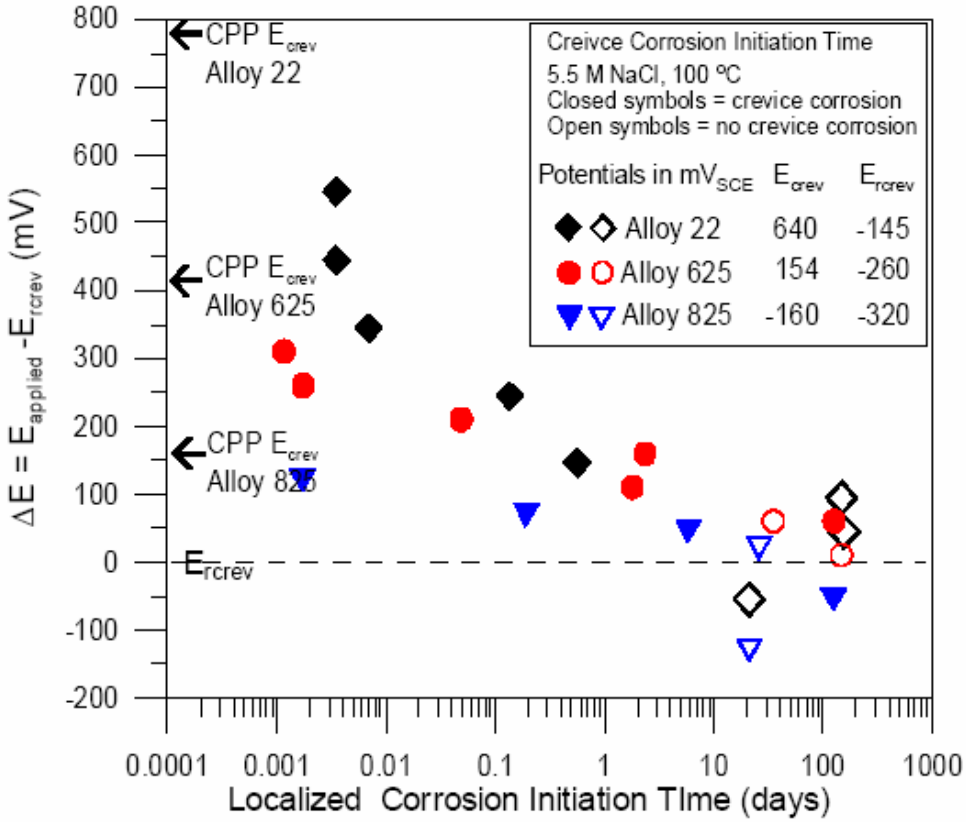
Basis for Overall Approach



- Initiation of stable localized corrosion is crucial for engineering structures
- Separation of problem into two components is valid at initiation

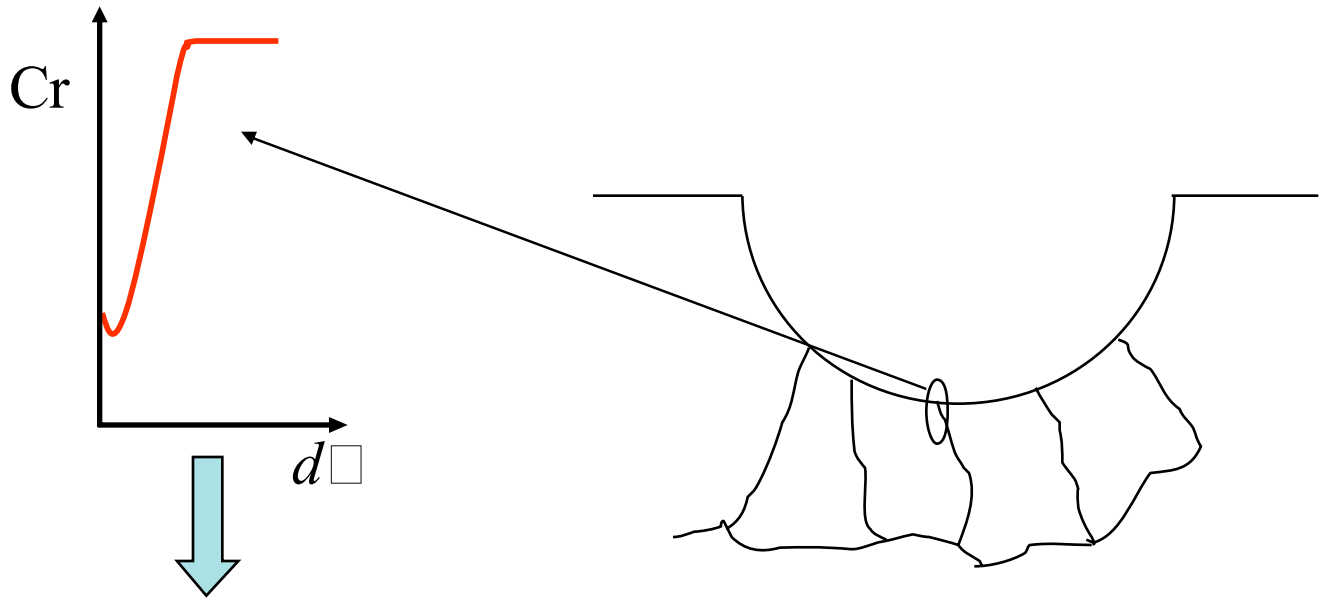
Validity of Repassivation Potential



- Localized corrosion initiates when E_{rp} is exceeded
- For industrial components, it is a good parameter for prediction when localized corrosion is likely to occur

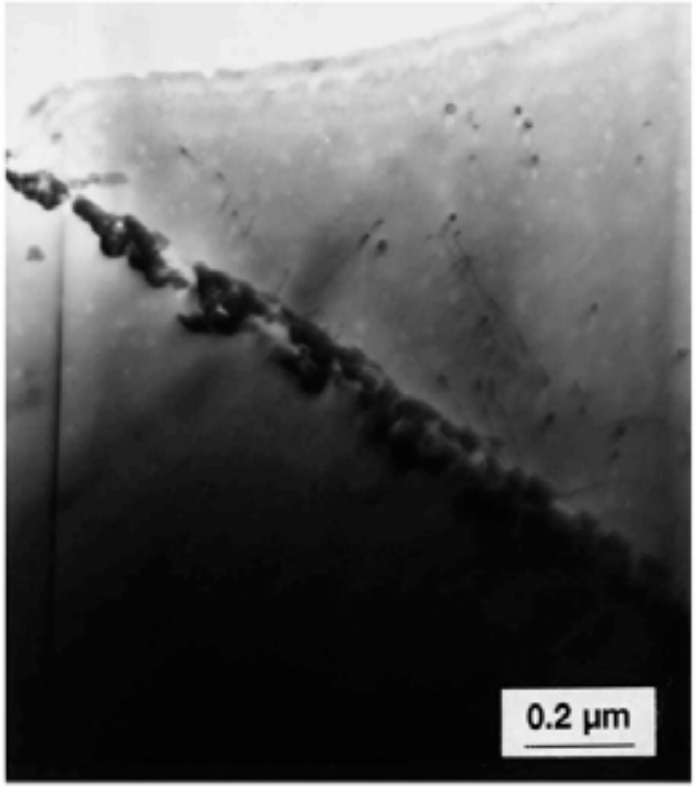
Dunn et al., Corrosion/2005

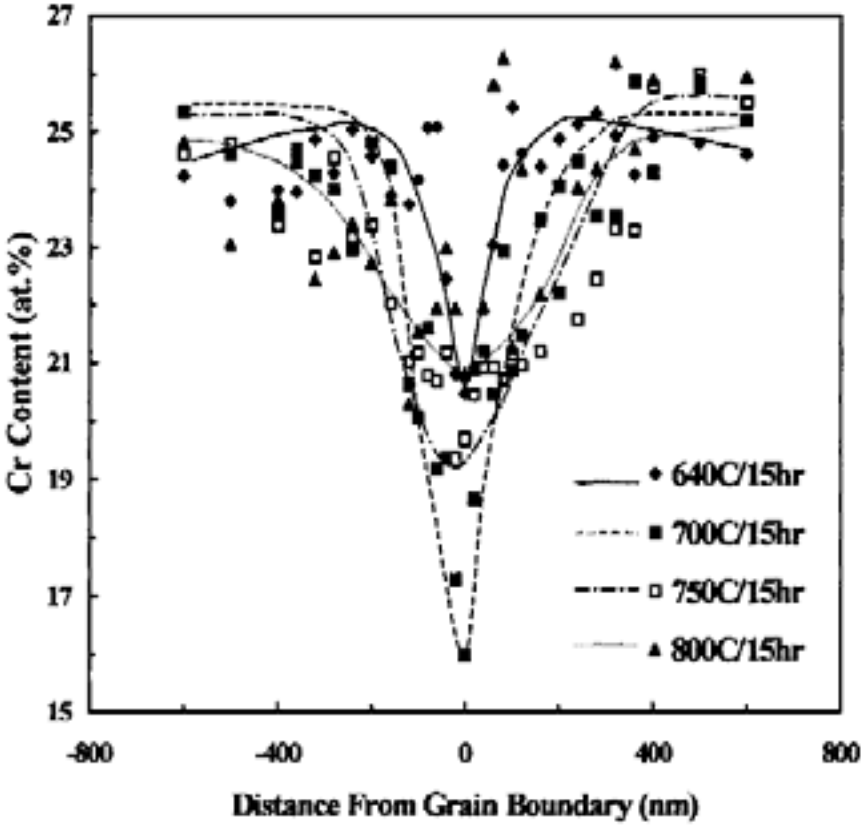
Modeling Heat Treatment Effects – A Conceptual Approach



Affects area-averaged dissolution and oxide rate parameters

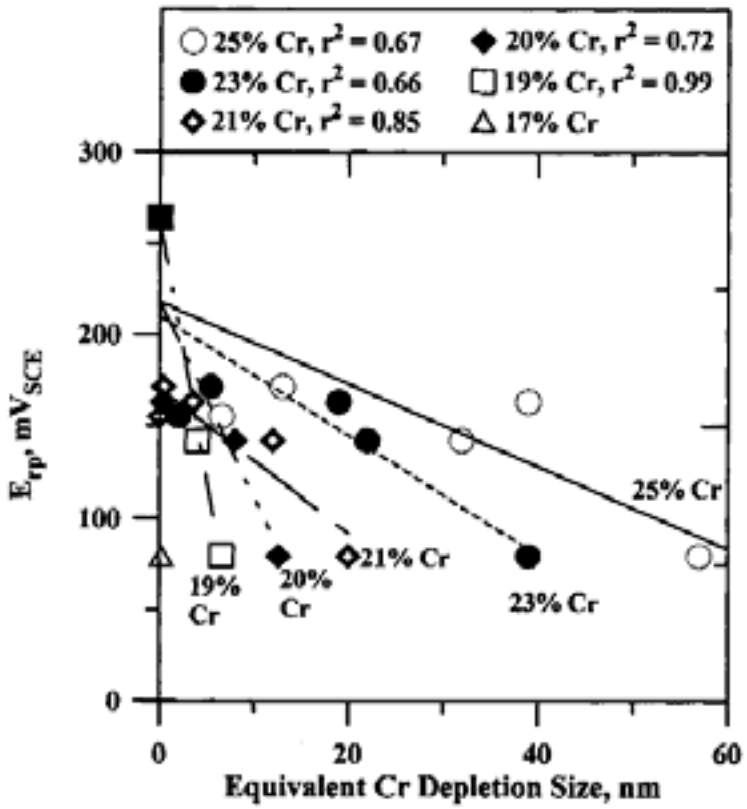
Effect of Heat Treatment on Microchemistry





Alloy 825: Pan et al., Met. Trans. (2000)

Effect of Heat Treatment on Corrosion

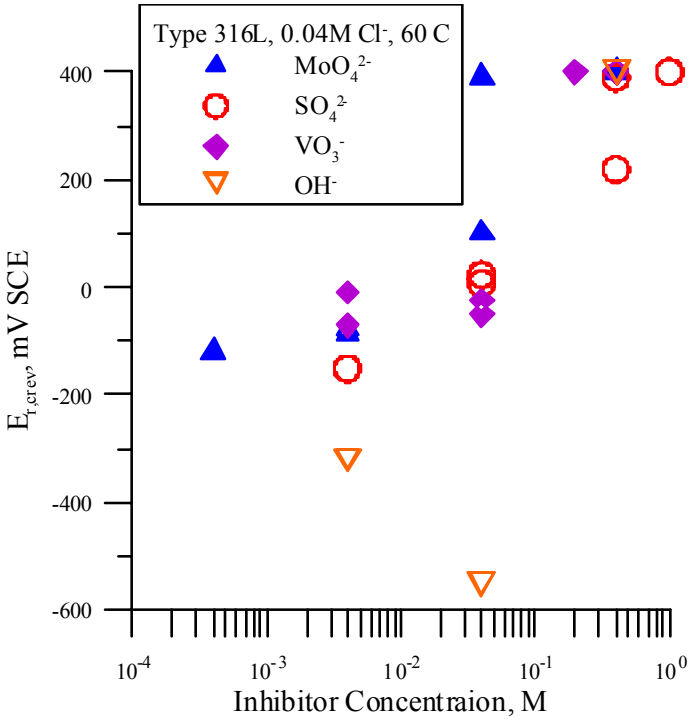


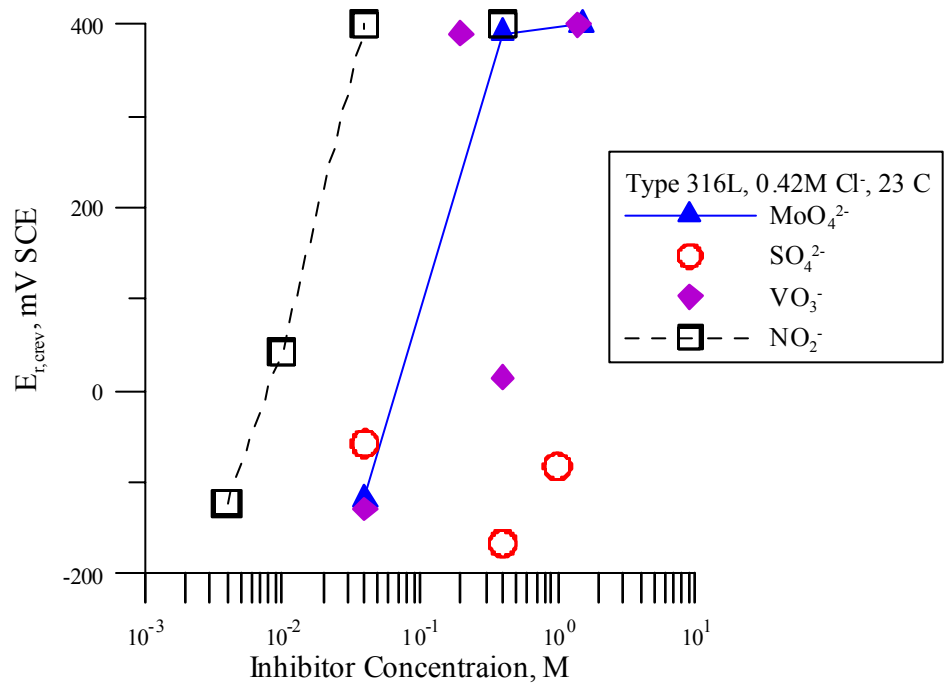
E_{rp} correlates with volume - averaged Cr level

Experimental Plan

- **Repassivation potential**
  - Effect of environmental variables
  - Effect of thermomechanical treatments
- **Corrosion potential**
  - Effect of environmental variables
- **Microchemistry data**
- **Pit propagation experiments**

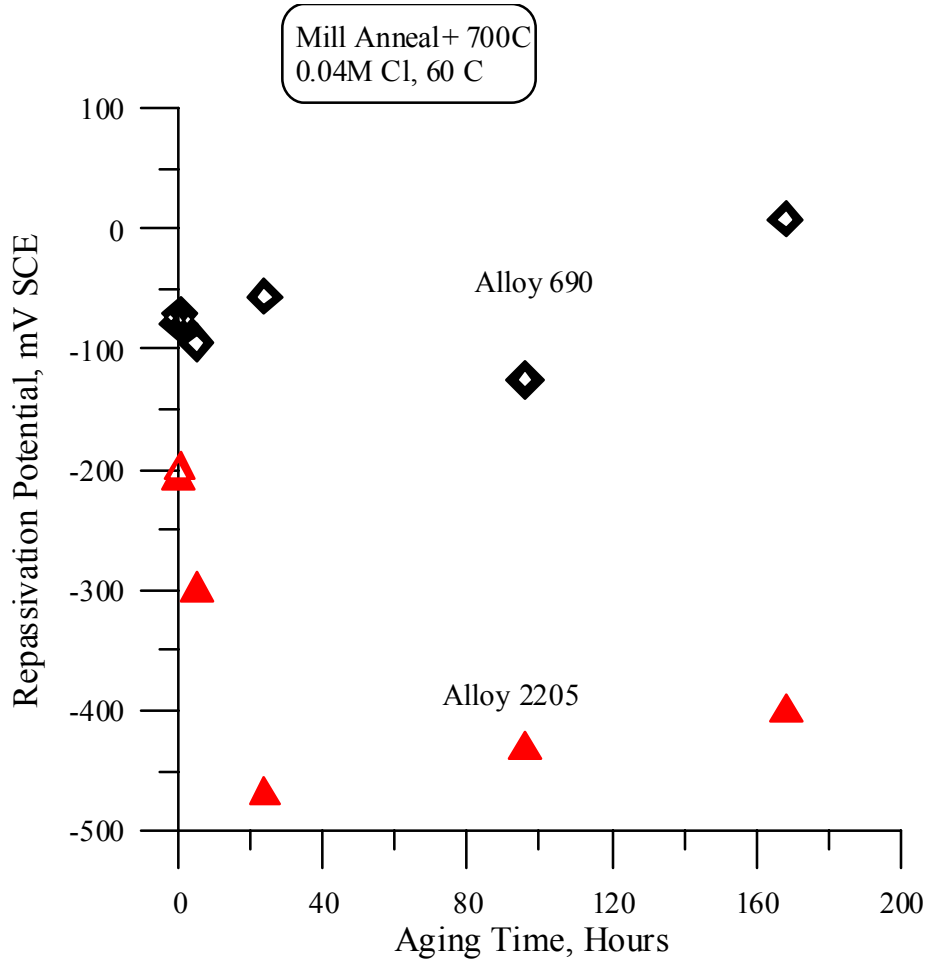
Effect of Environment





Inhibiting effect: $NO_3^- > MoO_4^{2-} > VO_3^- > SO_4^{2-} > OH^-$

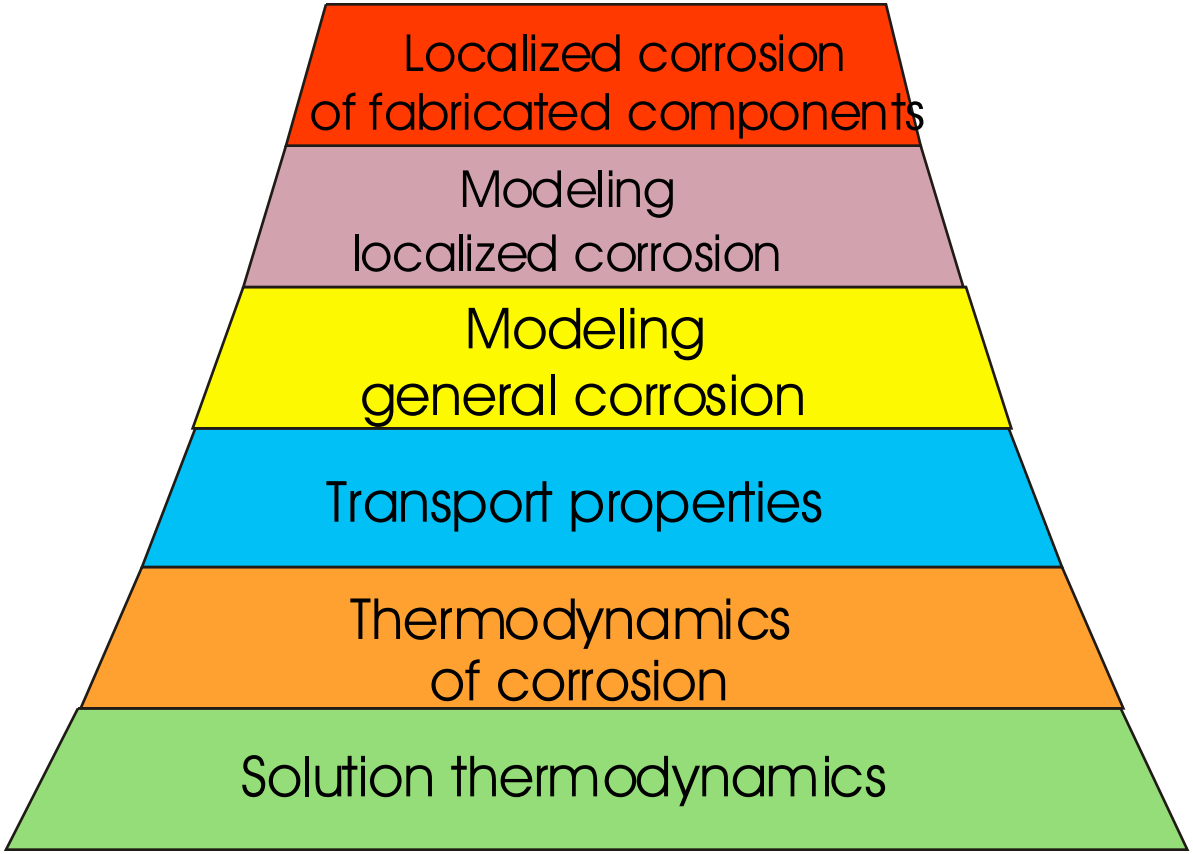
Effect of Heat Treatment



Summary of Experimental Database

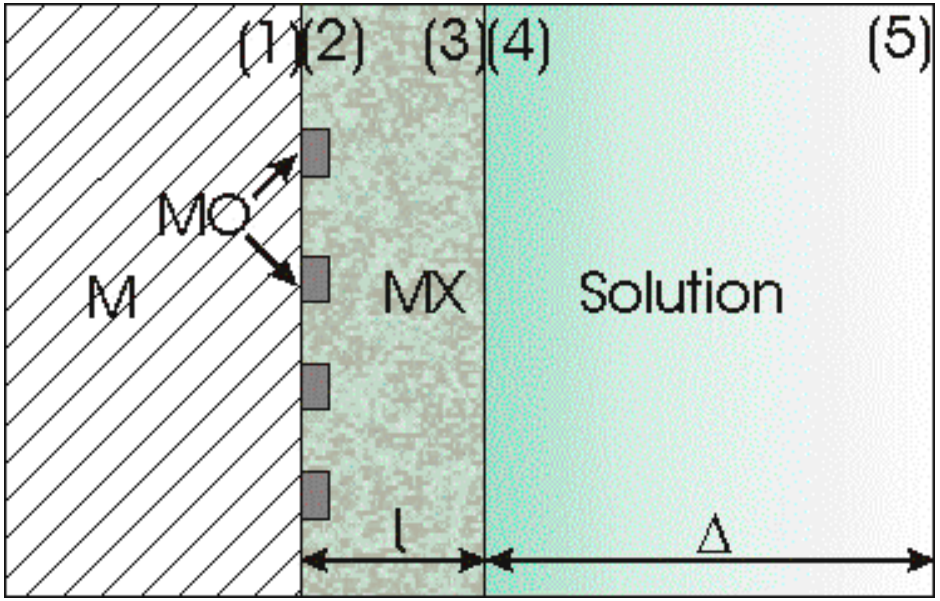
- Protection potentials established for multiple alloys
- Effects of heat treatments examined
- Corrosion potential measured as a function of oxygen concentration for two alloys
- Significant gaps and uncertainties in the data – need for further data generation

Structure of simulation technology for aqueous corrosion



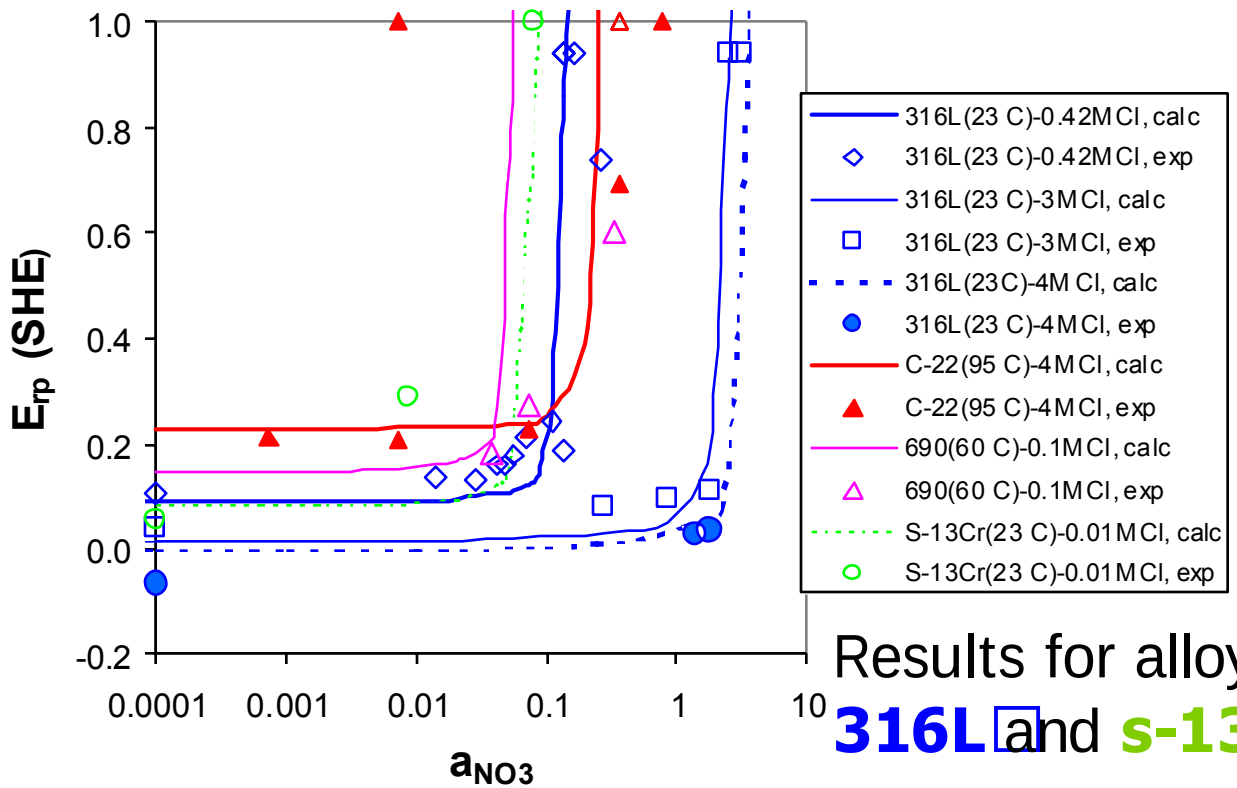
Predicting the repassivation potential:

Physical background of the model



- A closed-form solution can be found in the limit of repassivation
- It makes it possible to relate E_{rp} to solution chemistry and temperature

Generalized correlation for the repassivation potential of Fe-Ni-Cr-Mo-W alloys

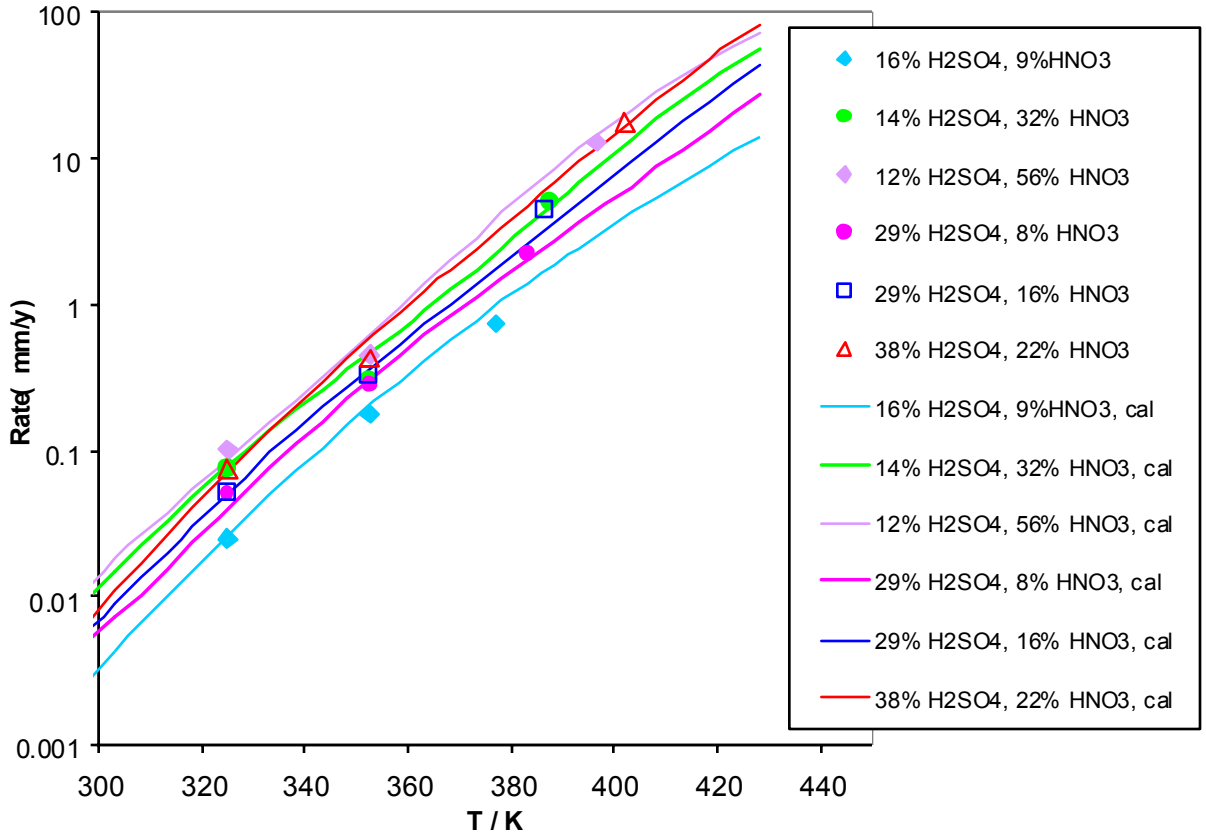


- Prediction of the inhibition effect of NO_3^- in Cl^- +NO_3^- mixtures at various temperatures

Results for alloys **C-22**, **690**, **316L** and **s-13Cr**

Prediction of general corrosion in mixed acids:

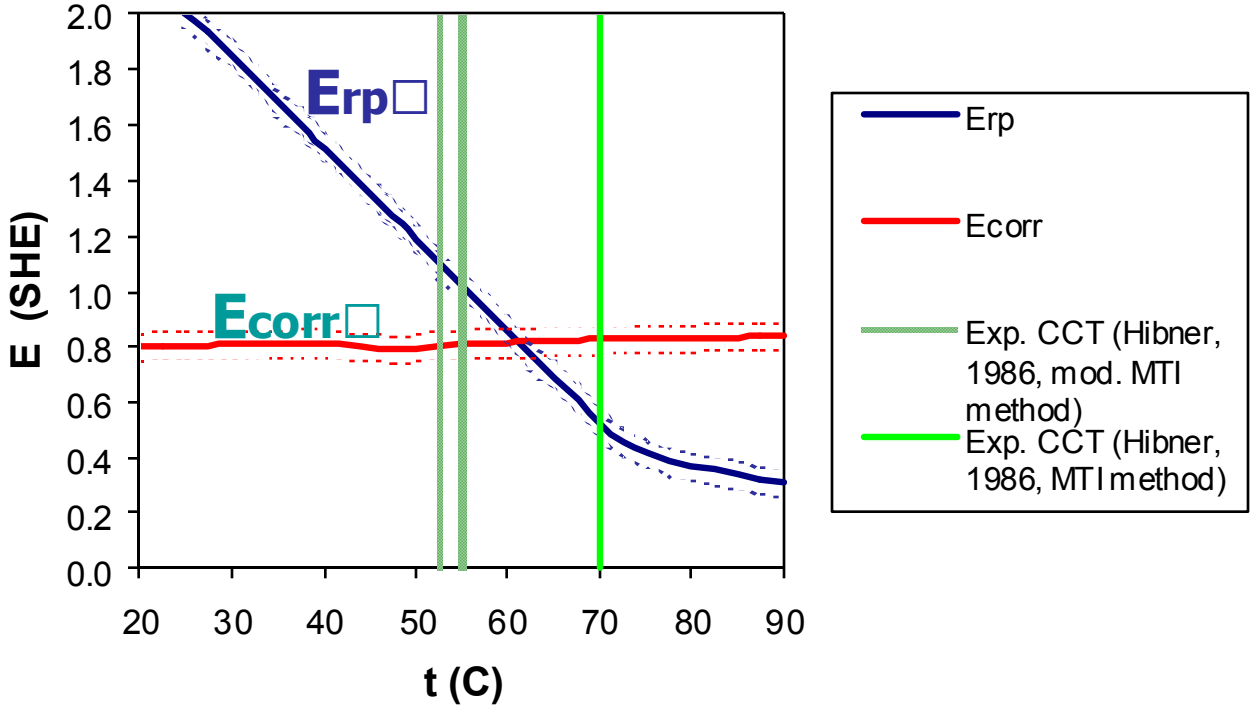
Alloy C-276 in H_2SO_4 + HNO_3



- Electrochemical parameters are derived only from data for pure acids
- Then, the model accurately predicts the rates in mixed acids

Verification of predictions against standard tests:

Predicting critical crevice temperature for alloy C-22 in 6% $FeCl_3$ solutions

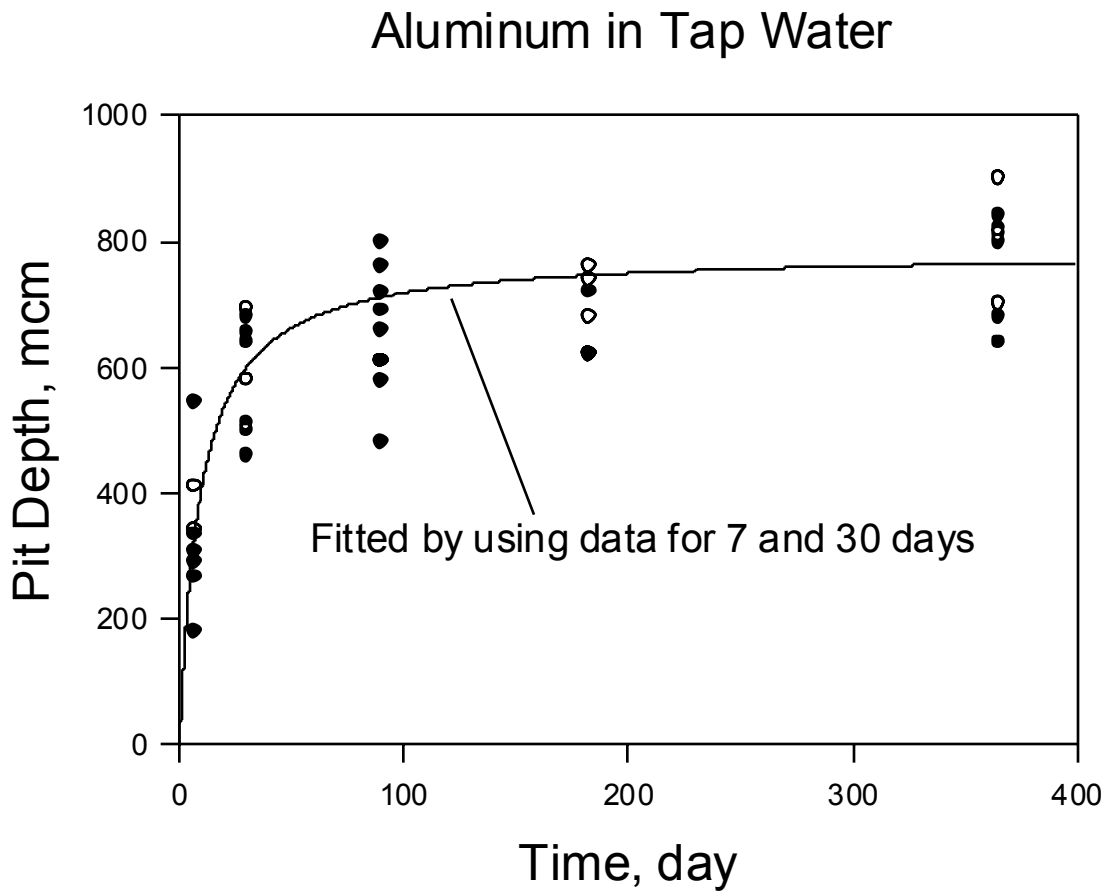


- Intersection of E_{corr} and E_{rp} corresponds to the critical crevice temperature
- Predicted CCT is in good agreement with experimental data

Extreme value statistics: Predicting corrosion damage

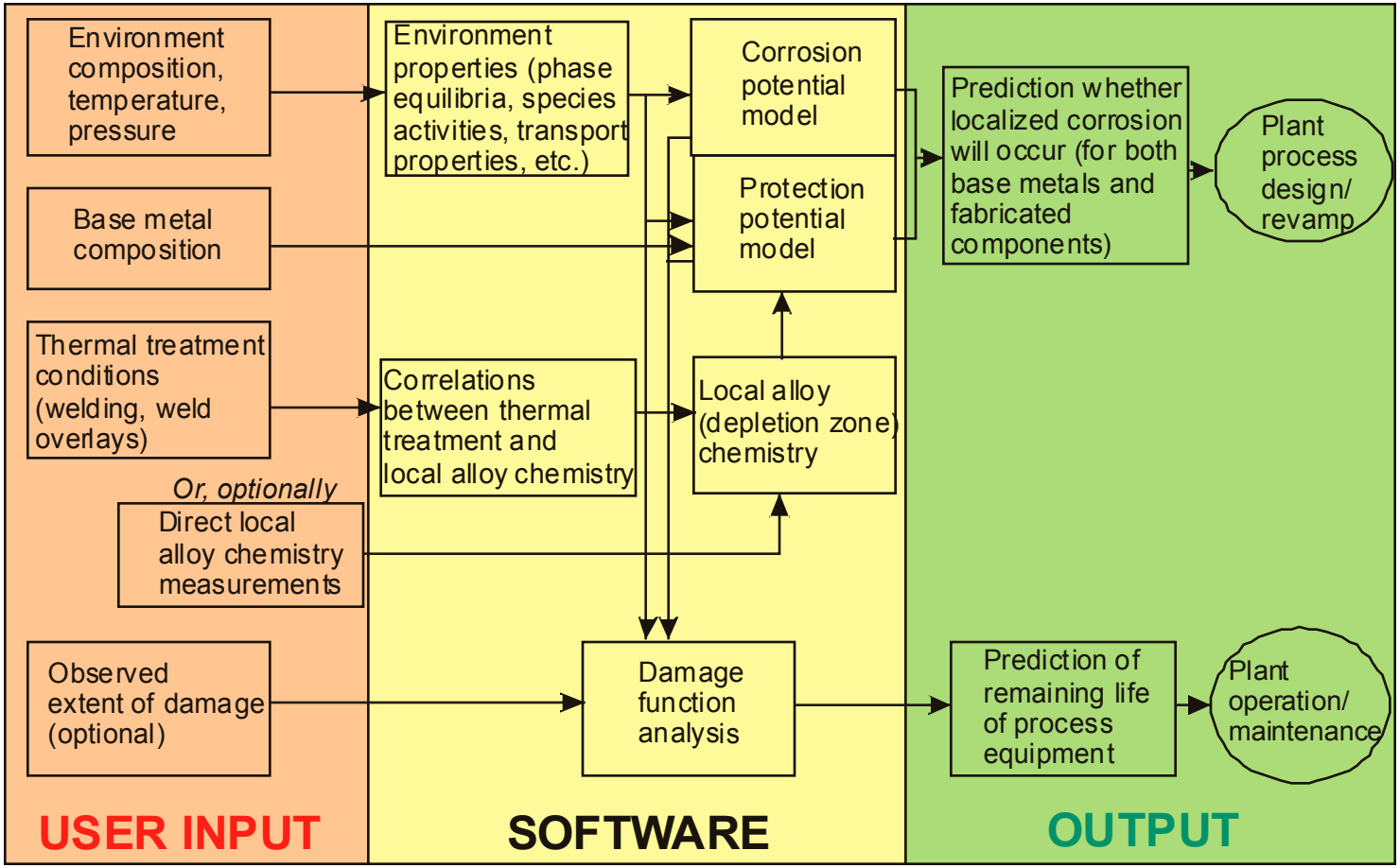
- ***Problem:*** Corrosion is observed in an existing installation. What is the probability of failure? How can we predict the useful lifetime of equipment?
- ***Approach:*** Combine extreme value statistics with fundamental corrosion models
- ***Benefit:*** Based on inspection data from short-term experiments, corrosion damage in the future can be predicted

Extreme pit depth versus exposure time for pitting



Only the data for t = 1 week and 1 month were used to fit parameters

Vision of localized corrosion software after three years



Major milestones to date

- A model has been established for predicting the occurrence of localized corrosion as a function of environment chemistry and temperature
- An experimental database has been established to elucidate the effects of aggressive and inhibitive species on localized corrosion
- The model has been comprehensively parameterized for both general and localized corrosion for alloys 22, 276, 625, 825, 600 and 690 in various aqueous environments (acids, bases, oxidizing species, inorganic inhibitors, etc.)
- A probabilistic model has been developed to predict long-term damage due to localized corrosion
- An interim version of CorrosionAnalyzer has been released (covering the six Ni-base alloys, carbon steel, Al, and four stainless steels (304, 316, 13%Cr and 254SMO)

Future plans (for the period 6/05 – 11/06)

- **Completion of experimental database**
  - Thermomechanical effects
    - Generate microchemistry data (collaboration with ORNL)
  - Other materials: G-35, Monel, 70-30, 90-10, exp. alloys
  - Pit growth studies
- **Extensions of modeling framework**
  - Development of a quantitative model for correlating electrochemical parameters with microchemistry, including heat treatment effects
  - Comprehensive treatment of inorganic inhibitors
  - Extension of electrochemical model to Cu-Ni alloys, Cu, Ni, duplex stainless steels
  - Extension of probabilistic prediction of corrosion damage (SCC)
- **Release of a fully commercial version of CorrosionAnalyzer**

Commercialization

- **Primary vehicle for commercialization: CorrosionAnalyzer software**
  - Currently used, in a preliminary form, by 32 software lessees (6 steering group members, 20 industrial users outside the steering group, 6 academic and research institutions)
  - Its capabilities will be dramatically enhanced as a result of this project

Commercialization pathways and risks

- **Establishing an effective channel to the market**
  - Existing worldwide network of agents and marketing partners
  - Existing client relationships with more than 80 companies in the chemical process industry
- **Technology transfer through industry groups, technical papers, professional association meetings**
- **Establishment of software training courses and dedicated customer technical support**
- **Application-specific projects, consulting and technical service**
- **Primary risks**
  - Crossing the education/information dissemination threshold
  - Proving value of corrosion simulation