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Scientific Consulting

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Mr. K. C. Chang
Mail Stop WF1-4H3
U. S. Nuclear Regulatory Commission
Washington, DC 20555

Dear Kien:

Services Rendered on High Level Waste Repository
Performance Assessment Development 3/13/88-3/26/88

During the referenced period I have continued to devote my attention to developing a practical procedure for incorporating the theoretical model of IGSCC into the CONVO. This effort has yielded significant results.

Modeling of IGSCC

One of the most important areas that requires analysis is the calculation of the activity of carbon in the 304L stainless steel. This activity is calculated according to the method presented by Natasen and Kassner[1]. The complex expression that they present contains a total of eight uncertain coefficients and 4 independent variables (the concentrations of C, Ni and Cr and the temperature T).

Using the experimental data provided by Natasen and Kassner, I have evaluated each of the coefficients and calculated their standard deviations. Also I have carried out a complete sensitivity analysis of their expression in order to determine the importance of the uncertainties in the coefficients and how the carbon activity is affected by variations in nickel, carbon and chromium concentrations and by temperature.

Based on this analysis it was possible to develop an approach that greatly simplifies the calculation without sacrificing any accuracy in the calculation. This result is a consequence of the fact that in the depletion zone where the precipitation of chromium takes place, the concentration of chromium may be treated as effectively constant. The sensitivity analysis shows

[1]Natesan, K. and T.F.Kassner, "Thermodynamics of Carbon in Nickel, Iron-Nickel and Iron-Chromium-Nickel Alloys", Met. Trans. 4 (1973) 2557-2566

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that the second order effect of carbon concentration on the carbon activity coefficient is small in comparison with the effects of nickel concentration and the uncertainties of the eight coefficients and may be neglected without sacrificing accuracy in the calculation.

Using these results it was possible to combine the eight coefficients into two coefficients which properly reflect the combined effects of the uncertainties of the original eight.

The result is the following expression for the carbon activity as a function of temperature, carbon concentration and nickel concentration:

$$\ln a_c = \ln\left(\frac{X_c}{1 - X_c}\right) + \left(-0.176 + \frac{0.608}{T}\right) \delta X_{Ni} + \left(a^* + \frac{b^*}{T}\right)$$

where $a^* = -0.469 \pm 0.439$
$b^* = 2.312 \pm 0.555.$

and δX_{Ni} is the expected variation in the concentration of nickel in different batches of alloy as determined by experiment.

This greatly simplified formulation will make it relatively simple to carry out the necessary Monte Carlo calculations and develop a response surface for this function.

The activity of chromium is also a complex temperature dependent function of the concentration of iron, nickel and carbon. I have begun a sensitivity analysis of this equation and anticipate that a similar simplification will be possible.

Other Information

I am enclosing three (3) copies of the Voucher for Professional services for your approval.

If you have any questions please feel free to call me.

Sincerely,

Robert B. Moler