**Simulating multi-component diffusion through a film of oxide**

This project is about setting up a multi-component diffusion equation and solving it in 1 dimension. You will have to write suitable code to do this.

You are probably familiar with the standard simple diffusion equation. There is a conserved flux ***j*** of something, particles per unit area per second perhaps, which depends on position and time It is proportional to the gradient in concentration *c* of the diffusing species according to

(1)

and

, (2)

which combine to give

. (2)

*D* is a diffusion coefficient. This equation is rather easy to solve, sometimes analytically. But the task here has some interesting twists. First, here’s the backstory. Oxidation of an aluminium-containing steel produces a film of crystalline alumina Al2O3 that grows by diffusion. Either the oxygen in the air diffuses through the growing film and forms fresh oxide at the metal-oxide interface, or the aluminium diffuses through the growing film and the fresh oxide grows at the outer surface of the film. The whereabouts of the fresh oxide can be determined experimentally, and both processes have been observed. This was achieved by interrupting the oxidation in air, in which the oxygen present is the isotope and then exposing the partially oxidised surface to the pure oxygen isotope instead. The distribution of the isotopes through the film was then examined, and the profile of was found to increase both towards the oxide – metal interface and towards the outer surface. We would like to simulate the system and study the distribution of fresh oxide and the rate of growth of the oxide film.

But here’s the first twist:

T1. Equations (1) and (2) have to be replaced by more general equations, because it’s believed that the oxygen (or aluminium) is mainly diffusing by a process in which the existing crystalline structure is not simply a static framework through which the oxygen atoms diffuse, it is an active participant in the process. In the simplest model, there are vacant oxygen lattice sites (denoted VaO) and aluminium lattice sites (denoted VaAl) and it is these that are the diffusing species.

Here's the second twist:

T2. Because the oxide film is growing, the boundaries between air to oxide and oxide to metal are actually moving. There are different ways of dealing with this, but it does not seem to have been addressed yet for this problem, and we should try and solve the moving boundary problem, at least approximately. There are a couple of methods we can try (to be discussed).

But that’s not all:

T3. Those vacancies I mentioned carry electric charges. For example, an aluminium ion carries the charge 3|e|, where |e| is the charge on an electron. If the ion is missing, the vacancy probably has an effective charge of -3|e| and we denote it . Similarly the oxygen vacancy would be Electric charges can build up at the interfaces and the resulting electric fields may accelerate or slow down the diffusion. Furthermore, to conserve charge there must be at least 2 kinds of diffusing species, so that for example an ionic current of could not be maintained indefinitely, they would eventually have to be balanced by a parallel current of electrons (or counter-current of holes) generated by the reactions at the interfaces.

There’s more than one way to tackle the modelling and the numerical solution of the resulting equations. A finite difference method can be tried, e.g. Euler, Crank-Nicolson or another implicit method, taking care to test the stability of the solution, or the problem can be formulated for solving by a phase-field method.

Particular questions to be considered:

1. Start with one species of vacancies and implement a solution for oxygen diffusion with no moving boundary.
2. Implement the moving boundaries, and try to establish an analytic criterion, in terms of D, when there is an effective steady-state solution. Can the growth rate be predicted without moving boundaries?
3. Include charged species and interface charges in the model and study their effect on the growth rate.