

MODELLING OXYGEN AVAILABILITY IN BLOOD SERUM, PERFLEUROCARBONS AND AQUEOUS BASED MEDIUM

[C.S.Kirk](#)¹ and [A.R.Mileham](#)²

¹*Depts. of Medical Sciences and Chemical Engineering, University of Bath, UK*

²*Dept. of Mechanical Engineering, Univ. of Bath, UK*

OVERVIEW: The finite volume method has been used in the simulation of atomic diffusion that typically occurs in high-temperature service conditions of post-weld heterogeneous welded joints in power generation plant. This paper reports on the algorithms that supported the investigation and describes their applicability to modelling the moving phase front and the related polymorphic cell used in the simulation of human cell behaviour, particularly applied to the examination of simulations for *in vitro* experiments using medium containing perfluorocarbons.

A study into the use of the Finite Volume Method to predict diffusion and carbide morphology in elevated temperature applications¹ enabled a better understanding of the complex rate reactions present in heterogeneous welds. This was primarily due to its rapid simulation output and increased grid density when compared with Finite Element Analysis.

The study was directed at welded joints which revealed that a carbon-depleted zone consisting of a ferrite rich, alloy impoverished zone that was susceptible to cracking after welding and which increased in size, with time. This methodology has been applied to the availability of oxygen from oxy-haemoglobin surrounded by blood serum and from oxygen enriched (relative to water) perfluorocarbon medium which can be used in certain types of *in vitro* experiment. This methodology enables a better understanding of the transfer mechanisms where rates of transfer are diffusion limited and permits simulation of experimental conditions over a range of oxygen or nutrient values including applicability to aqueous based medium.

CONCLUSION: By studying various decomposition models it was possible to derive a similar methodology for the decomposition front considered to be in the form of a moving wave front for oxygen concentrations in oxygen rich medium. It is proposed that the moving surface boundary methodology be adapted and used to model the decomposition of both perfluorocarbons at minimal velocity and to give better understanding of the transfer mechanisms occurring *in vivo* from red

blood cells at full flow and restricted flow in or adjacent to capillary beds. This methodology may be extended to provide a basis for considering perfluorocarbons at velocities approaching *in vivo* conditions and, similarly hypoxic medium.

An equation first applied to modelling metallurgical events was revised to assist practitioners in developing reasoning for the dimension of the moving boundary dimension. This is a modified 'Fick' equation, being :

$$x^2 = \frac{C_c - C_d}{C_b} 2D_i t \quad (1)$$

where reference is made to the solubility concentrations in various human or laboratory fluids. The chemical composition of the fluid/material determines diffusion before the diffused element reaches any interface. It may be concluded that a reaction coefficient depends on composition (available for diffusion), temperature, solubility and diffusivity but not on any type of dissimilar material combinations. Transport across areas may also be subject to dynamic cell morphology.

REFERENCES: ¹ Kirk, C.S., and Mileham, A.R., (2001), Modelling Diffusion in Heterogeneous Transition Welds using e Finite Volume Method, EPSRC Research Report and Assessment, University of Bath, 2001.