**s8b.m3.p3** **Flat model bulk solvent correction in the program *REFMAC*** R.A.Steiner[#] and G.N. Murshudov[§*]. [#]*Department of Biophysical Chemistry, University of Groningen Nijenborgh 4, 9747 AG Groningen, the Netherlands;* [§]*York Structural Biology Laboratory, University of York Heslington, York, United Kingdom, e-mail: garib@ysbl.york.ac.uk*
Keywords: methods crystallography, refinement, modelling.

Bulk solvent correction based on simple flat bulk solvent model has been implemented in the program REFMAC[1].

Our work takes advantage of the results of Jiang[2] who showed that the flat solvent model works surprisingly well despite its simplicity and that correction is not substantially improved by considering the solvent distributed in radial shells. The model based on $F_o$-$F_c$ map seems to overfit the diffraction data.

Incorporation of structure factors from the flat bulk solvent reduces on average $R_{free}$ values of about 0.3% when compared to corrections based on the Babinet principle alone. As expected low resolution data benefit most from the inclusion of bulk solvent correction. Efficient bulk solvent correction has also been performed utilising a model based on 2m$F_o$-D$F_c$ map. A prerequisite for all models is the generation of an accurate mask for the solvent accessible regions.

The current first implementation assigns a constant density value at grid points in the solvent allowed space and its Fourier transform is used as partial structure. The bulk solvent is assumed to be constituted by free water molecules. A possible improvement of this assumption is that to use form factors based on local ordered structure. Water molecules for example are likely to form a net with tetrahedral nodal points.

At this stage not yet interpreted but ordered parts of the unit cell are still included in the bulk solvent region. $2F_o$-$F_c$ or experimental maps could be analysed to distinguish them from pure bulk solvent. They should be treated separately as their contributions to structure factors are different.

[1] Murshudov, G.N., Vagin, A.A and Dodson, E.J. (1997). Refinement of macromolecular structures by the maximum-likelihood method. *Acta Cryst.* D**53**, 240-255.
[2] Jiang, J.S. and Brünger, A.T. (1994). Protein hydration observed by X-ray diffraction. *J.Mol.Biol.* **243**, 100-115.