Instructions for use of HardSPEC Calibration Module

The calibration parameters developed for the HardSPEC model to simulate wash-off of compounds from specific surfaces were based on results from a set of 'Controlled wash-off Studies' carried out using 6 test substances (see Shepherd & Heather, 1999a & b). However some of these parameters, particularly those to simulate processes specific to very soluble compounds, were based on very limited data (Hollis *et al*, 2017, Appendix 3) and are thus less robust than most of the other calibration parameters. As a result, a 'Calibration Module' for the model was developed to enable users to improve this aspect of model predictions based on measured data from an appropriate compound-specific Controlled Wash-off Study. This module has been added as a separate worksheet in the Excel-based model, titled "Calibration Module".

The Calibration Module should only be used in conjunction with compound-specific measured data from an appropriate Controlled Wash-off Study. If you believe that a Controlled Wash-off study is required for the substance you wish to register for use on hard surfaces, please contact HSE at CRD.Information.Management@hse.gov.uk for further information.

Before moving to the Calibration module, users should add all relevant compound data to the "Herb Props" worksheet as described in section 5.1 of the latest Guidance Document (Hollis *et al*, 2017).

Calibration is then carried out in up to 4 steps using the "Calibration_module" worksheet:

1. Step 1 is to add the mass applied (mg) to each 0.54 m^2 of surface type to cell E12, the volume of each wash-off sample collected and the measured mass (mg) lost in that volume to Cells B16 to B36 & D16 to D36, respectively. Calibration cannot proceed without these data.

2. In Step 2, you start by calibrating Kp asphalt. In the "Calibrated values" cell (L17), enter the value given in the 'Default values' cell to the left (K17). A 'Difference' value and a 'Percentage difference' value will appear in cells M17 and merged cells OPQ17. Then, in the top menu of Excel, go to "*Data*", select "*What-If Analysis*" and choose "*Goal Seek*". In the dialogue box, enter the cell M17 in the *'set cell*' option, the value 0.0 in the '*To value*' option and the cell L17 in the '*By changing cell*' option. Press OK. When the Goal Seek function has finished, if it finds an optimum value for Kp, it will tell you "found a solution" and an optimized Kp surface value will appear in the 'Calibrated values' cell L17. Click on the OK option. **Note that the optimized value may be negative, which is not valid for Kp. If this happens you should change the negative value in cell L17 to 0.** If Goal Seek cannot 'improve' on the Kp value that was entered originally, it will say "may not have found a solution", in which case click on the Cancel option and make a note of the default value of Kp. Repeat this procedure for Kp concrete. When you have optimized Kp for both surfaces, proceed to Step 3.

3. In step 3, you calibrate the soluble loss reduction functions. Start with asphalt surfaces and go to the 'Calibrated values' cell O33. In cell O33, type the value given into the 'Default values' cell to the left (N33) and a 'Model Efficiency' value will appear in cell P33. Select

the Goal Seek function as you did in step 2 and in the dialogue box, enter the cell P33 in the '*set cell*' option, the value 1.0 in the '*To value*' option and the cell O33 in the '*By changing cell*' option. Press OK. Goal Seek will try to optimize the model efficiency value to an ideal of 1.0. When it has finished, if it finds an optimum value for the model efficiency it will tell you "found a solution" and an optimized Xasphalt constant value will appear in the 'Calibrated values' cell O33. Click on the OK option and note the Model Efficiency value that appears in cell P33/34. If it cannot 'improve' on the model efficiency value resulting from the default value that was entered originally, it will say "may not have found a solution", in which case click on the Cancel option, enter the 'Default' value from cell N33 into the adjacent cell O33 and the default Model Efficiency value will appear in cell P33/34. Go to the next calibration value down, in row 34 and repeat the procedure. Repeat this for each of the calibration parameters in cells rows 35 & 36. Finally, repeat the procedure again for the two Calibration parameters for concrete surfaces in cells in rows 38 & 39. Proceed to Step 4.

4. In the final calibration step 4, you optimize the desorption routines for wash-off. Depending on compound physico-chemical properties and the mass applied, these may not always be activated in the model, but calibration is still necessary. Start with asphalt surfaces and go to the 'Calibrated values' cell O52. In cell O52, type in the value given in the 'Default values' cell to the left (N52) and a 'Model Efficiency' value will appear in cell P52/53. Select the Goal Seek function and follow the Goal Seek procedures as you did in step 3. Once you have optimized this calibration parameter, do the same for the next one down (row 53) and also for the two concrete parameters in rows 55 & 56. When step 4 is complete, you have finished calibration of the model. Make a note of the final Model Efficiency values for both asphalt (in cell P52/53) and concrete (in cell P55/56).

References

J.M. Hollis, C.T. Ramwell, I.P. Holman and M.J. Whelan. (2017). HardSPEC - A First-tier Model for Estimating Surface- and Ground-Water Exposure resulting from Herbicides applied to Hard Surfaces. Updated Technical Guidance on Model Principles and Application for version 1.4.3.2.
Appendix 3. Calibration of the surface wash-off and ballast leaching sub-models. *https://www.hse.gov.uk/pesticides/pesticides-registration/data-requirements-handbook/fate/hardspec/HardSPEC_Guidance_Appendices.pdf*

A.J Shepherd and A.I.J. Heather, (1999a). Factors affecting the loss of six herbicides from hard surfaces. Soil Survey and Land Research Centre report for the Department of Environment Transport and Regions, 55 pp.

A. Shepherd and A.I.J. Heather, (1999b). Factors affecting the loss of six herbicides from hard surfaces, in Proc XI Symp Pesticide Chemistry: Human and environmental exposure to xenobiotics, September 11–15 Cremona, Italy, ed by Del Re A.A.M., Brown C., Capri E., Errera G., Evans S.P. and Trevisan M., La Goliardica Pavese, Pavia, pp 777–784.