Optimisation of Process Equipment using Global Surrogate Models

D. W. Stephens[1] and P.D. Fawell[2]
[1]Applied CCM Pty Ltd, [2]Parker Centre (CSIRO Process Science and Engineering)

Introduction

The computational cost associated with the use of high- fidelity CFD models poses a serious impediment to the successful application of optimisation algorithms in engineering design. Evaluation of such models may take significant computational time for complex geometries. In many design problems, thousands of function evaluation may be required to undertake an optimisation study. As a result, CFD models are often impractical for design optimisation. In contrast, surrogate models are compact and cheap to evaluate (order of seconds or less) and can, therefore, be easily used for such tasks.

Case Study – Sediment transport in a Thickener

The aim of this study was to:

- build a surrogate model from the CFD model of material transport generated by raking in a thickener, detailed in [1], and
- to use the surrogate to investigate optimum rake blade angle and speed.

The rake geometry is illustrated in Figure 1. The CFD output quantities total torque and a measure of plug flow were used for the surrogate building. The plug flow metric is calculated as the residence time standard deviation divided by the mean residence time for plug flow. An example of the graphical output from the model is shown in Figure 2.

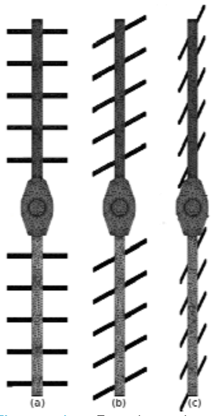

Figure 1: Example rake blade configurations, (a) 0°, (b) 30 and (c) 65°.

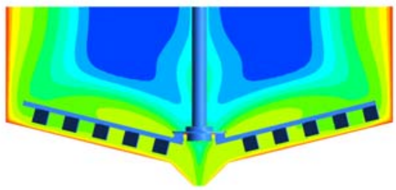

Figure 2: Residence time contours on a plane through the rake (rake speed 1.25 rpm, blade angle 30º). Ten linearly distributed colour bands of blue to red from 0 to 4000 s. In this case study, the system was a 2 m diameter pilot thickener, 2 m high with a 14° floor angle. The rake was comprised of two arms, each with 5 equi-spaced blades, on a 75 mm diameter rake shaft. The blade angle could be varied from 0-65°. Each blade was 290 × 75 mm and they were positioned with a gap of 23 mm between the blade and the thickener floor. Slurry is fed into the thickener through a ring manifold at a rate of 3 m3 h-1. The slurry is non-Newtonian with the rheology being input as a rheogram determined from experiments.

Results

Surrogate Building

All of the RBF (Radial Basis Function) surrogate models (one for each CFD output quantity) were built using the SUrogate MOdelling (SUMO) MATLAB toolbox[2] with the toolbox flow control illustrated in Figure 3. Surrogate accuracy assessment was performed using a 20-fold cross-validation.

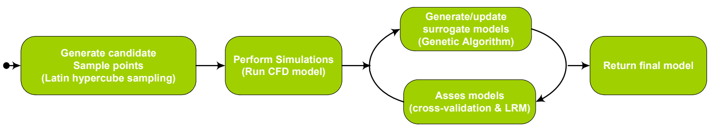

Figure 3: SUMO toolbox flow control used for building the RBF surrogates.

Optimisation – Single composite objective function

The case study is a multi-objective optimisation problem with two competing objectives – minimise rake torque and maximise the plug flow behaviour. This can be framed as a single objective function problem using combinations of the individual objective functions. Contour plots of three composite objective functions with different preferences for each of the individual objective functions are shown in Figure 4.

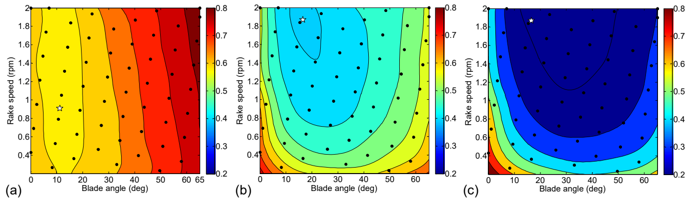

Figure 4: Contour plots showing the three different objective functions and the optimum value (white star) for (a) 80:20, (b) 50:50 and (c) 20:80 preference to torque and plug flow metric, respectively.

Optimisation – Multiple objective functions

In multi-objective optimisation problems there are many solutions where a trade-off between objective functions exists. Such trade-off (optimal) solutions provide a clear front (Pareto-optimal) when plotted in objective space. Not all rake designs will lie on the Pareto-optimal front; in fact there are often more sub-optimal configurations than optimal. In multi-objective optimisation the task is to find the set of solutions that define the Pareto-optimal-front by considering all objectives to be important.

Rather than using multi-objective optimisation algorithms as discussed by Deb[3], a novel approach is taken here for finding the Pareto-optimal front. The surrogate model is evaluated at many different design variable combinations to generate the objective space feasible region. The Pareto-optimal front is located on the boundary of this region. For this case, a grid comprising of 2600 input point combinations was evaluated for each of the objective functions, with the total evaluation time being less than 1 minute. The objective function values for each of these input points can be plotted in objective space (blue diamonds), as shown in Figure 5, with the Pareto-optimal front marked by the red line.

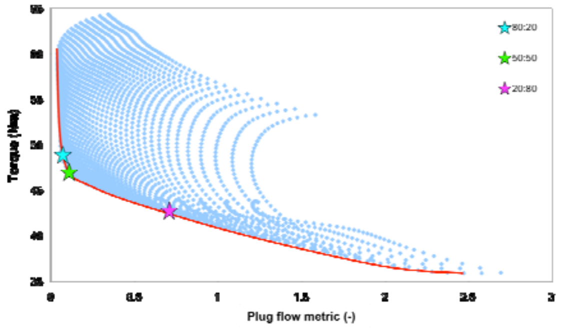

Figure 5: Responses for the rake transport case study plotted in objective space with the Pareto-optimal front marked by the red line. The coloured stars on this line indicate the locations of the three optimal solutions found using the different composite objective functions.

Conclusion

Output from a CFD model of sediment transport in a raked thickener was used to produce surrogate models representing rake torque and plug flow behaviour. Examples were provided demonstrating how these surrogate models can be used to optimise the rake design using both a single and multiple objective functions.

It must be stressed that surrogate models are only as good as the underlying CFD model from which they are created.

References

[1] RUDMAN, M., SIMIC, K., PATERSON, D.A., STRODE, P., BRENT, A. and SUTALO, I.D.(2008). "Raking in gravity thickeners", *International Journal of Mineral Processing*, **86**, 114-130.

[2] GORISSEN, D., CROMBECQ, K. COUCKUYT, I., DHAENE, T. and DEMEESTER, P. (2010). "A surrogate modelling and adaptive sampling toolbox for computer based design", Journal of Machine Learning Research, **11**, 2051-2055.

[3] DEB, K. (2005). "Multi-objective Optimisation", In BURKE, E.K. and KENDALL, G. (Eds.), *Search methodologies: Introductory tutorials in optimization and decision support techniques*. Berlin: Springer-Verlag, pages 273-316.

Acknowledgements

This work was conducted via the AMIRA project P266F: "Improving Thickener Technology". The authors acknowledge the financial support given to this research from the project sponsors.

Contact: Darrin Stephens
Phone: (03) 8376 6962
Email: d.stephens@appliedccm.com.au
Web: http://www.appliedccm.com.au

Applied CCM