Publications November 2012

Madden, A.; Whittle, M.; Ford, N.; Eaglestone, B. Difficulties with Internet searches by the general public: their nature, and the response of searchers. Submitted to J. Doc.

Refereed Journal Publications

Articles with an asterisk have been submitted as part of a research assement exercise.

Whittle, M., Quegan, S., Uryu, Y., Michael Stüewe,Yulianto, K.
Detection of tropical deforestation using ALOS-PALSAR: A Sumatran case study.
Remote Sensing of Environment. **124**, 83-98 (2012)

Whittle M.; Travis K.P. Dynamic Simulations of colloids by core-modified dissipative particle dynamics. J. Chem. Phys. **132**, 124906-124916 (2010)

*Whittle, M., Eaglestone, B., Ford, N., Gillet, V.J., Madden, A.D. Data Mining of Search Engine Logs. Journal of the American Society for Information Science and Technology. 58(14), 2382-2400, (2007).

Whittle, M., Eaglestone, B., Ford, N., Gillet, V.J., Madden, A.D. Query Transformations and their role in web searching by the general public. Information Research, 12(1) paper 276, October 2006. [Available at http://InformationR.net/ir/12-1/paper276.html]

Whittle, M.; Gillet, V.J.; Willet, P.; Loesel, J. Analysis of Data Fusion Methods in Virtual Screening: Similarity and Group Fusion. J. Chem. Inf. Model. 46, 2206-2219 (2006).

*Whittle, M.; Gillet, V.J.; Willet, P.; Loesel, J. Analysis of Data Fusion Methods in Virtual Screening: Theoretical Model. J. Chem. Inf. Model. 46, 2193-2205 (2006).

Whittle, M.; Gillet, V.J.; Willet, P.; Loesel, J; Alexander, A. Enhancing the Effectiveness of Virtual Screening by Fusing Nearest-Neighbour Lists: A Comparison of Similarity Coefficients. J. Chem. Inf. Comput. Sci. 44, 1840-1848 (2004).

*J. D. Holliday, N. Salim, M.Whittle[‡], P. Willett. Analysis and Display of the Size Dependence of Chemical Similarity Coefficients. J. Chem. Inf. Comput. Sci. 43, 819-828, (2003).
[‡] Principle author.

Whittle, M.; Willett, P.; Klaffke, W.; van Noort, P. Evaluation of Similarity Measures for Searching the Dictionary of Natural Products Database. J. Chem. Inf. Comput. Sci. 43, 449-457, (2003).

M. Whittle, E. Dickinson. Research Note On Simulating Colloids by Dissipative Particle Dynamics: Issues and Complications. J. Colloid and Interface Sci. 242, 106-109, (2001).

Martin Whittle, Brent S. Murray, Jianshe Chen and Eric Dickinson. Simulation and Experiments on Colloidal Particle Capture in a Shear Field. Langmuir, 16, 9784-9791,(2000).

Martin Whittle, Brent S. Murray and Eric Dickinson. Simulation of Colloidal Particle Scattering: Sensitivity to Attractive Forces. Journal of Colloid and Interface Science, 225, 367 , (2000).

Martin Whittle, Brent S. Murray, Eric Dickinson and Valerie J. Pinfield. Determination of Interparticle Forces by Colloidal Particle Scattering: A Simulation Study. J. Coll. and Interface Sci. **223**, 273-284, (2000).

M. Whittle and E. Dickinson. Pore Size in Model Particle Gels. Molecular Physics, **96**, 259-264, (1999).

Whittle M, Atkin RJ, Bullough WA. Dynamics of a Radial Electrorheological Clutch. International Journal of Modern Physics B 13: 2119-2126 (1999).

M. Whittle, E. Dickinson. Large Deformation Rheological Behaviour of a Model Particle Gel . J. Chem. Soc., Faraday Trans., **94**, 2453-2462, (1998)

*M. Whittle and E. Dickinson. Stress Overshoot in a Model Particle Gel. J. Chem. Phys. **107**, 10191-10200, (1997)

M. Whittle and E. Dickinson. Brownian Dynamics Simulation of Gelation in Soft Sphere Systems With Irreversible Bond Formation. Molecular Physics 90, 739, (1997).

M. Whittle, R. J. Atkin, and W. A. Bullough. Dynamics of an ER valve. Int. J. of Modern Physics B. 10, 2933-2950, (1996).

M. Whittle, R. J. Atkin, and W. A. Bullough. Fluid Dynamic Limitations on the Performance of an Electrorheological Clutch. J. of Non–Newtonian Fluid Mechanics, 57, 61-81, (1995).

M. Whittle, R. Firoozian, D. J. Peel and W. A. Bullough. Electrorheological Relaxation Times Derived from Pressure Response Experiments in the Flow Mode. J. of Non–Newtonian Fluid Mechanics, 57, 1 - 25, (1995).

M. Whittle, W. A. Bullough, D. J. Peel and R. Firoozian. The Dependence of Electrorheological Response on Conductivity and Polarization Time. J. of Phys E, **49** (6), 5249-5259, (1994).

M. Whittle, R. Firoozian, W. A. Bullough and D. J. Peel: Pressure Coupling in the Electrical Response of Electrorheological Valves. Int. J. of Modern Physics B. **8**, 2903 - 2919, (1994).

M. Whittle, R. Firoozian, D. J. Peel and W. A. Bullough. Decomposition of the pressure response in a ER Valve Control System: J. Intelligent Material Systems and Structures, **5**,105-111,(1994).

M. Whittle, R. Firoozian, W. A. Bullough and D. J. Peel. A model for the electrical characteristics of an ER valve. Int. J. of Modern Physics B. **6** (15/16), 2683-2704, (1992).

M. Whittle and A. J. Masters. Liquid crystal formation in a system of fused hard spheres. Molecular Physics, 72, 247-265, (1991).

M. Whittle. Computer simulation of an electrorheological fluid. J. of Non–Newtonian Fluid Mechanics, 37, 233-263, (1990).

M. Whittle and J. H. R. Clarke. Force and torque correlations in diatomic fluids. Molecular Physics 51, 1253-1267, (1984).

M. Whittle and J. H. R. Clarke. Shear viscosity in diatomic fluids. Molecular Physics, 49, 1199-1208, (1983).

M. Whittle and J. H. R. Clarke. Nitrate ion reorientation in aqueous Calcium Nitrate solutions: new evidence for ion association. Chemical Physics Letters, **98** (2), 172-175, (1983).

M. Whittle and J. H. R. Clarke. Ionic reorientational motions in aqueous solutions: a depolarised light scattering study of NO3- and SCN-. Molecular Physics, **44**, 1435-1451, (1981).

Conference Papers

M. Whittle, R.J. Atkin and W.A. Bullough. Dynamics of a Radial Electrorheological Clutch. *Proceedings of the International Conference on Electrorheological Fluids, Yamagata, Japan.* pp641 - 648, (1997).

A. Hosseini- Sianaki, W. A. Bullough, M. Whittle, R. C. Tozer and J. Makin. : Steady State and Transisent Models for the Electical Response of and Electro-rheological catch system. *Proceedings of the International Conference on Electrorheological Fluids, Yamagata, Japan*. pp649 - 660, (1997).

M. Whittle, R. J. Atkin, and W. A. Bullough : The Dynamics of an ER valve. *Proceedings of the International Conference on Electrorheological Fluids, Sheffield.* (1996). Ed. W.A. Bullough, World Scientific Publishing Co. Pte. Ltd.

M. Whittle, R. Firoozian, W. A. Bullough and D. J. Peel : Pressure Coupling in the Electrical Response of Electrorheological Valves. *Proceedings of the International Conference on Electrorheological Fluids, Feldkirch* (1993), pp100 - 117. Ed. R.Tau, World Scientific Publishing Co. Pte. Ltd..

M. Whittle, R. Firoozian, D. J. Peel and W. A. Bullough: Generalised Pressure Responses of Electro-Rheological Valves in the Steady State, Time and Frequency Domains. *Proceedings of the 2nd Minsk International Heat and Mass Transfer Forum, MIF-92, Minsk, Byelarus* (May 1992) pp 151-160.

M. Whittle, R. Firoozian, D. J. Peel and W. A. Bullough : A model for the electrical characteristics of an ER valve. *Proceedings of the International Conference on Electrorheological Fluids, Carbondale* (1992), pp343-346. Ed. R.Tau, World Scientific Publishing Co. Pte. Ltd..

M. Whittle, R. Firoozian, W. A. Bullough and D. J. Peel : The Pressure Response in ER Valve Flow, *Proceedings of conference: Recent Advances in Adaptive and Sensory Materials and their Application.* April 27-29 (1992) pp495 - 505. Blacksburg, Virginia, (Technomic)

Other Publications and as Contributing Author

Martin Whittle, Valerie J. Gillet and Peter Willett
A Simulation Study of the Use of Similarity Fusion for Virtual Screening
Huma Lodhi, Yoshihiro Yamanishi (editors). Chemoinformatics and Advanced Machine Learning Perspectives: Complex Computational Methods and Collaborative Techniques (IGI Book Series: Advances in Chemoinformatics and Computational Methods); Chapter 4; IGI Global, 2010. ISBN 978-1-61520-911-8 (hardcover) -- ISBN 978-1-61520-912-5 (ebook).

Nigel Ford, Barry Eaglestone, Andrew Madden and Martin Whittle. Web searching by the “general public”: and individual differences perspective. Journal of Documentation, 2009, 65(4), 632-667.

Kirstin Moffat,Valerie J. Gillet,, Martin Whittle, Gianpaolo Bravi, and Andrew R. Leach. A Comparison of Field-Based Similarity Searching Methods: CatShape, FBSS, and ROCS. *J. Chem. Inf. Model.* **2008,** *48,* 719–729

Semenova M.G.; Chen J.S.; Dickinson E.; Murray B.S. & Whittle M. Sticking of protein-coated particles in a shear field. Colloids and Surfaces B-Biointerfaces **22** (3): 237-244 (2001).

Dickinson, E.; Murray, B. S.; Whittle, M. & Chen, J. (2001) Dynamic interactions between adsorbed protein layers from colloidal particle scattering in shear field. In *Food Colloids, Fundamentals of Formulation*, Dickinson, E. & Miller, R. (Eds.), Royal Society of Chemistry, Cambridge, pp. 272 – 281.

H. Casanova, J. Chen, E. Dickinson, B. S. Murray, P. V. Nelson & M. Whittle; Dynamic colloidal interactions between protein-stabilised particles – experiment and simulation. Phys. Chem. Chem. Phys., **2**, 3861-3869, (2000)

C.M. Wijmans, M. Whittle and E. Dickinson, "Structure and Rheology of Simulated Particle Gel Systems" in "Food Emulsion and Foams: Interfaces, Interactions and Stability", eds. E. Dickinson and J.M. Rodríguez Patino, Royal Society of Chemistry: Cambridge, pp. 342-355 (1999).

B.S. Murray, E. Dickinson, J. M. McCarney, P. V. Nelson and M. Whittle: Observation of the Dynamic Interaction Forces between Casein-Coated Latex Particles. Langmuir **14**, 3466-3469, (1998).

A. Hosseini- Sianaki, W. A. Bullough, M. Whittle, R. C. Tozer and J. Makin.: Steady-State and Transient Models for the Electical Response of and Electro-rheological catch system. *IEE Proc.-Sci. Meas. Technol.*, **145**, (3), 94-100, (1998).

A. Hosseini- Sianaki, W. A. Bullough, R. C. Tozer, M. Whittle and J. Makin : Experimental Investigation into the Electrical Modelling of Electrorheological Fluids in the Shear Mode. *IEE Proc.-Sci. Meas. Technol.*, **141**, 531-537, (1994).

A. J. Masters and M. Whittle: The Application of Some Reference Theories to the Hard Spheroid Fluid. *Journal of Chemical Physics*, **99**, 6205, (1993). See also **105**, 3892, (1996).

M. Whittle and W. A. Bullough: The Structure of Smart Fluids : News & Views, *Nature*, **358,** 373, (1992)

M. Whittle: Modelling two-phase fluids.*Physics World*, **2**, 39, (1989).

M. Whittle: Review of the sixth CCP5 meeting.*Information Quarterly for MD & MC Simulations* **5**, 4-12, (1982).

M. Whittle: Non-equivalence of step and delta function in perturbation experiments.*Information Quarterly for MD & MC Simulations* **5**, 14-16, (1982).

Journal Reviewing

Over the last few years I have refereed articles submitted to the following journals:

Journal of Physical Chemistry
Recent Patents on Materials Science
Journal of Physics: Condensed Matter
Applied Rheology
Journal of Chemical Information & Modeling
ACM Transactions on Information Systems
ACM Transactions on the Web (TWEB)
Journal of Micromechanics and Microengineering

Smart Materials & Structures

Presentations at International Conferences

The 6th Information Seeking in Context Conference (ISIC), Sydney, Australia, 19-21 July, 2006.
Presentation: Query Transformations and their role in web searching by the general public.

CCP5 Workshop on Long Range Forces in Simulation (Hydrodynamics and electrostatics) Daresbury Laboratory (15th December 2000).
Presentation: Simulations of colloidal particle scattering using the multi-subunit method.

The 10th International Conference on Colloid and Interface Science. Organised by IACIS. Bristol UK (23-28th July 2000).
Presentation: Simulations of Colloidal Particle Scattering.

CECAM workshop on Hydrodynamic interactions, Lyon, France (April 1997)
Presentation: Brownian Dynamics Simulation of Gels.

Colloidal Aspects of Complex Fluids organised by the Colloidal and Interface Science Group of the Royal Society of Chemistry. Cambridge (26-28 March 1996).
Presentation: Brownian Dynamics Simulation of Gelation in Soft Sphere Systems with Irreversible Bond Formation.

The 5th International Conference on Electrorheological Fluids, Sheffield, UK (10-14th July 1995).
Presentation: Pressure Response in Electrorheological Valves.

Material Research Society Spring Meeting, San Francisco, USA, (March 1995)
Presentation: Theoretical Acceleration Limit of Electrorheological Clutches.

International Symposium on Viscoelastic Fluids, Tobago WI (4-6th January 1994). Visit Sponsored by the Royal Academy of Engineering.
Presentation: Dynamics of ER fluids Derived from Pressure Response Experiments in the Flow Mode.

The 4th International Conference on Electrorheological Fluids, Feldkirch, Austria (20-23rd July 1993).
Presentation: Pressure Coupling in the Electrical Response of ER Valves.

The 2nd Minsk International Heat and Mass Transfer Forum, MIF-2, Minsk, Byelarus (May 1992). Visit sponsored by the Royal Society.
Presentation: The Pressure Response in an ER Valve.

The 3rd International Conference on Electrorheological Fluids, Carbondale USA (October 1991).
Presentation : A Model For the Electrical Characteristics of an ER valve.

Poster Presentations

The Third Joint Sheffield Conference on Chemoinformatics, Sheffield, UK (21st-23rd April 2004).
Title: Why Size Matters and the Tanimoto Coefficient Works.
Martin Whittle, Naomie Salim, John Holliday and Peter Willett.

The Sixth International Conference on Chemical Structures, Noordwijkerhout, The Netherlands (2–6th June 2002).
Title: Virtual screening of Natural Product Databases by Similarity Searching and Data Fusion.
Martin Whittle, Peter Willett, Werner Klaffke and Paula van Noort

The 10th International Conference on Colloid and Interface Science, IACIS. Bristol (23-28th July 2000).
Title: Interparticle Forces by Colloidal Particle Scattering (II). M. Whittle, Brent S. Murray and E. Dickinson.

Faraday Discussions No. 112. Chester (12-14th April 1999).
Title: Interparticle Forces by Colloidal Particle Scattering (I). M. Whittle Brent S. Murray, E. Dickinson and V.J. Pinfield.