ANDREW HASLAM

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SUMMARY

- **Ph.D. in Physical Chemistry**; 17 years experience as Research Associate and Fellow.
- **RESEARCH:**
  - **statistical thermodynamics and phase equilibria**
    - industrial **gas-polymer** systems
    - **liquid-crystal** systems
    - role of **intermolecular potentials** and their influence on mixtures and phase equilibria
  - **thermodynamics in relation to energy and the environment**
    - **electrolyte systems** – including brines and mixtures with non-electrolytes, such as CO_2
    - **organic Rankine cycles**, and related devices for the conversion of waste heat to useful energy
  - **flow assurance**
    - thermodynamic modelling of **gas hydrates** for application in reservoir / flow simulations
    - thermodynamic modelling of **asphaltene** and heavy-oil systems
  - **simulation of fluids and solids**
    - atomistic (**molecular dynamics** (MD) and **Monte Carlo** (MC)) and **mesoscale** (coarse-grained MD and kinetic-MC / finite-element) simulations of systems ranging from generic Lennard-Jones fluid to **polymers** and **metals**
    - **adsorption** of fluids on solid surfaces
    - multiscale and hierarchical simulations; serial and parallel platforms
- **TEACHING**:
  - class tutorials in **thermodynamics** with undergraduate chemical engineers (10 years)
  - graduate lecture course: *An Introduction to Statistical Thermodynamics and its Application in Equation-of-State Modelling of Fluids*
  - supervision of research students: lectures in **simulation** and **statistical mechanics**; short courses in UNIX and FORTRAN programming; general advice and assistance
  - laboratory demonstrating and lectures in **physical chemistry** to undergraduate chemists

APPOINTMENTS

Imperial College London, UK, Department of Chemical Engineering
- ***Research Fellow (Molecular Systems Engineering group)*** ..... *August 2008 to date*

Imperial College London, UK, Department of Chemical Engineering
- ***Research Associate (Molecular Systems Engineering group)*** ..... *October 2004 – July 2008*

Argonne National Laboratory, USA, Materials Science Division
- ***Visiting Scientist (Interfacial Materials Group)*** ..... *June 2004 – October 2004*

Imperial College London, UK, Centre for Process Systems Engineering
- ***Research Associate (Molecular Systems Engineering group)*** ..... *August 2001 – June 2004*

Argonne National Laboratory, USA, Materials Science Division
- ***Research Associate (Interfacial Materials Group)*** ..... *February 1999 – July 2001*

University of Illinois at Chicago, USA, Department of Chemical Engineering
- ***Research Associate*** ..... *January 1998 – January 1999*

University of Sheffield, UK, Department of Chemistry and
University of Patras, Greece, Department of Physics
- ***Research Associate*** ..... *May 1997 – January 1998*

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EDUCATION

Ph.D. in Physical Chemistry, University of Sheffield, UK, Dept. of Chemistry .....*March 1997*

- *Monte Carlo simulation study of hard-sphere chain polymers*.
  - Advisors: Prof. George Jackson and Prof. Tom McLeish

B.Sc. in Chemistry (1st class, honours), University of Sheffield, UK *1992*

B.Sc. in Mathematical Sciences, University of Birmingham, UK *1984*

(Details of early education ('O' and 'A' levels) are given at the end of this document.)

REFEREED JOURNAL PUBLICATIONS

1. A.J. Haslam, G. Jackson and T.C.B. McLeish, *An investigation of the shape and crossover scaling of flexible tangent hard-sphere polymer chains by Monte Carlo simulation*, 1999, J. Chem. Phys., **111**, 1, 416–428.
2. A.J. Haslam, G. Jackson and T.C.B. McLeish, *A Monte Carlo study of the induced deformation of polymer chains dissolved in stretched networks*, 1999, Macromolecules, **32**, 21, 7289–7298.
3. A.J. Haslam, S.R. Phillpot, D. Wolf, D. Moldovan and H. Gleiter, *Mechanisms of grain growth in nanocrystalline fcc metals by molecular-dynamics simulation*, 2001, Mat. Sci. and Eng. A, **318**, 293–312.
4. A.J. Haslam, S.R. Phillpot, D. Wolf, D. Moldovan and H. Gleiter, *Combined atomistic and mesoscale simulation of grain growth in nanocrystalline thin films*, 2002, Comp. Mater. Sci., **23**, 15–32.
5. D. Moldovan, D. Wolf, S.R. Phillpot and A.J. Haslam, *Mesoscopic simulation of two-dimensional grain growth with anisotropic grain-boundary properties*, 2002, Phil. Mag. A, **82**, 1271–1297.
6. D. Moldovan, D. Wolf, S.R. Phillpot and A.J. Haslam, *Role of grain rotation in grain growth in a columnar microstructure by mesoscale simulation*, 2002, Acta. Mater., **50**, 3397–3414.
7. A.J. Haslam, V. Yamakov, D. Moldovan, D. Wolf, S.R. Phillpot and H. Gleiter, *Stress-enhanced grain growth in a nanocrystalline material by molecular-dynamics simulation*, 2003, Acta Mater., **51**, 2097–2112.
8. A. Galindo, A.J. Haslam, S. Varga, G. Jackson, A.G. Vanakaras, D.J. Photinos and D.A. Dunmur, *The phase behavior of a binary mixture of rodlike and disclike mesogens: Monte Carlo simulation, theory, and experiment*, 2003, J. Chem. Phys., **119**, 5216–5225.
9. A.J. Haslam, D. Moldovan, V. Yamakov, D. Wolf, S.R. Phillpot and H. Gleiter, *Effects of grain growth on grain-boundary diffusion creep by molecular-dynamics simulation*, 2004, Acta Mater., **52**, 1971–1987.
10. A.J. Haslam, N. von Solms, C.S. Adjiman, A. Galindo, G. Jackson, P. Paricaud, M.L. Michelsen and G.M. Kontogeorgios, *Predicting enhanced absorption of light gases in polyethylene using simplified PC-SAFT and SAFT-VR*, 2006, Fluid Phase Equilib. **243**, 74–91.
11. G.N.I. Clark, A.J. Haslam, A. Galindo and G. Jackson, *Developing Optimal Wertheim-like Models of Water for use in Statistical Associating Fluid Theory (SAFT) and related approaches*, 2006, Mol. Phys. **104**, 3561–3581
12. M.A. Franco-Melgar, A.J. Haslam and G. Jackson, *A generalisation of the Onsager trial-function approach: Describing nematic liquid crystals with an algebraic equation of state*, 2008, Mol. Phys. **106**, 649–678.
13. A.J. Haslam, A. Galindo and G. Jackson, *Prediction of binary intermolecular potential parameters for use in modelling fluid mixtures*, 2008, Fluid Phase Equilib. **266**, 105–128.
14. B.P. Ló, A.J. Haslam and C.S. Adjiman**,** *An algorithm for the estimation of parameters in models with stochastic differential equations*, Chem. Eng. Sci., 2008, **63**, 4820–4833.
15. M.A. Franco-Melgar, A.J. Haslam and G. Jackson, *Advances in generalised van der Waals approaches for the isotropic–nematic fluid phase equilibria of thermotropic liquid crystals – an algebraic equation of state for attractive anisotropic particles with the Onsager trial function*, 2009, Mol. Phys. **107**, 2329–2358.
16. P.-A. Artola, F.E. Perreira, C.S. Adjiman, A. Galindo, E.A. Müller, G. Jackson and A.J. Haslam, *Understanding the fluid phase behaviour of crude oil: asphaltene precipitation*, Fluid Phase Equilib. 306 (2011) 129–136.

17. S. Dufal, A. Galindo, G. Jackson and A.J. Haslam, *Modelling the effect of methanol, glycol inhibitors and electrolytes on the equilibrium stability of hydrates with the SAFT-VR approach*, Mol. Phys. 110 (2012) 1223–1240.

18. J. Jover, A.J. Haslam, A.Galindo, G. Jackson and E.A. Müller, *Pseudo hard-sphere potential for use in continuous molecular-dynamics simulation of spherical and chain molecules*, J. Chem. Phys. 137 (2012) 144505.

19. H. Dominguez, A.J. Haslam, G. Jackson and E.A. Müller, *Modelling and understanding of the vapour-liquid and liquid-liquid interfacial properties for the binary mixture of n-heptane and perfluoro-n-hexane*, J. Molec. Liq. 185 (2013) 36–43.

20. R.M. Horton, A.J. Haslam, A. Galindo, G. Jackson and M.W. Finnis, *New methods for calculating the free energy of charged defects in solid electrolytes*, J. Phys. Condens. Matt. 25 (2013) 395001.

21. O.A. Oyewunmi, A.I. Taleb, A.J. Haslam and C.N. Markides, *An Assessment of Working-Fluid Mixtures using SAFT-VR Mie for Use in Organic Rankine Cycle Systems for Waste-Heat Recovery*, Comp. Thermal Sci., (2014); *accepted*.

22. J.M.A. Schreckenberg, S. Dufal, A.J. Haslam, C.S. Adjiman, G. Jackson and A. Galindo, *Modelling of the thermodynamic and solvation properties of electrolyte solutions with the statistical associating fluid theory for potentials of variable range*, Mol. Phys. (2014)*; accepted*.

23. E. Forte, A.J. Haslam, G. Jackson and E.A. Müller, *Effective coarse-grained solid-fluid potentials and their application to model adsorption of fluids on heterogeneous surfaces*, Phys. Chem. Chem. Phys., (2014); *accepted*.

(24. O.A. Oyewunmi, A.I. Taleb, A.J. Haslam and C.N. Markides, *On the Use of SAFT-VR Mie for Assessing Fluorocarbon Working-Fluid Mixtures in Organic Rankine Cycles for Waste-Heat Recovery*, ASME J. Eng. Gas Turbines Power 2014; *under peer review*.)

PUBLICATIONS: BOOK CHAPTERS

1. D. Moldovan, D. Wolf, S.R. Phillpot and A.J. Haslam*, Grain rotation as a mechanism of grain growth in nanocrystalline materials*, Chapter 2 in ICASE/LARC Interdisciplinary Series in Science and Engineering 9: *Trends in Nano-Scale Mechanics: Analysis of Nanostructured Materials and Multi-Scale Modeling*, pp 35–59, V.M. Harik and M.D. Salas (Eds), Kluwer Academic, The Netherlands, 2003**.**

2. B.P. Ló, A.J. Haslam, C.S. Adjiman, and M. Laso, *A method for the systematic estimation of parameters for a stochastic reptation model*, Part I Chapter 3 in *Multiscale Modelling of Polymer Properties*, M. Laso and E.A. Perpète (Eds), Computer-Aided Chemical Engineering 22, Elsevier, 2006.

3. A.J. Haslam, Ø. Moen, C.S. Adjiman, A. Galindo and G. Jackson, *Design of polyolefin reactor mixtures*, Part II Chapter 6 in *Multiscale Modelling of Polymer Properties*, M. Laso and E.A. Perpète (Eds), Computer-Aided Chemical Engineering 22, Elsevier, 2006.

PUBLICATIONS: CONFERENCE PROCEEDINGS ETC

1. D. Moldovan, D. Wolf, S.R. Phillpot and A.J. Haslam, *Multiscale Simulation of Grain Growth in Nanocrystalline Thin Films*, in: *Multiscale Modeling, Simulation and Visualization and Their Potential for Future Aerospace Systems*, Ahmed K. Noor (compiler), 299–330, 01 July 2002, NASA CP-2002-211741; proceedings of the workshop held March 5-6, 2002, NASA Langley Research Center, Hampton, VA, USA.

2. D. Moldovan, A.J. Haslam and D. Wolf, *Multiscale Simulation of Grain Growth in Nanocrystalline Materials*, 2003, in *Computational Fluid and Solid Mechanics 2003*, K.J. Bathe (Ed.) (proceedings of the second M.I.T. Conference held in Boston, USA, June 2003), pp. 482–485.

3. A.J. Haslam, V. Yamakov, D. Moldovan, D. Wolf, S.R. Phillpot and H. Gleiter, *Stress-enhanced grain growth in nanocrystalline materials*, in: Advances in Science and Technology Vol.44, Proceedings of the Special Symposium *Modeling and Simulating Materials Nanoworld* (Part C), of the 3rd International Conference *Computational Modeling and Simulation of Materials*, part of CIMTEC Conferences, Acireale, Sicily, Italy, May 30–June 4, 2004.

4. B.P. Ló, A.J. Haslam and C.S. Adjiman, *Parameter estimation for stochastic differential equations: algorithm and application to polymer melt rheology*, Proceedings of 16th European Symposium on Computer Aided Process Engineering, 9–13 July 2006.

PAPERS IN PREPARATION

S. Dufal, T. Lafitte, A.J. Haslam, A. Galindo and G. Jackson, *The A in SAFT: investigating the association contributions within a Wertheim TPT1 treatment*, (completed and awaiting PI approval for submission).

S. Dufal, T. Lafitte, A.J. Haslam, A. Galindo and G. Jackson, *Developing potential models for use with the SAFT-VR Mie Equation of State*, (completed and awaiting PI approval for submission).

J. Jover, A.J. Haslam, A. Galindo, G. Jackson and E. A. Müller, *Study of the demixing of an athermal colloid-polymer mixture*, (completed and awaiting PI approval for submission).

P.E. Brumby, H.H. Wensink, A.J. Haslam and G. Jackson, *Structure and interfacial tension of a hard-rod fluid in planar confinement*, (completed and awaiting PI approval for submission).

J.F. Jover, E.A. Müller, A.J. Haslam, A. Galindo, G. Jackson, H. Toulhoat and C. Nieto-Draghi, *An examination of the aggregation behaviour of coarse-grained molecular models of asphaltenes*, (completed and awaiting PI approval for submission).

PRESENTATIONS

1. A. J. Haslam and G. Jackson, *Computer simulations of polymers and polymer networks*, Molecular Organisation in Thin Films Meeting, Sheffield, 16 May 1994.

2. A. J. Haslam, G. Jackson and T. C. B. McLeish, *Simulation of a simple-model polymer in an aligned network* (talk and poster), 14th Experimental Thermodynamics Conference, Reading, Berks., UK, 6 April 1995.

3. A. J. Haslam, S. C. McGrother, R. P. Sear and G. Jackson, *Ordering in dipolar, associating, and polymeric systems*, 3rd EC Network Meeting on Molecular Organisation in Liquid Crystals Resulting from Particular Intermolecular Interactions, Thorpe, Derbyshire, 21 May 1995.

4. A. J. Haslam, G. Jackson and T. C. B. McLeish, *Monte Carlo simulations of polymers and polymer networks using a continuum model* (poster), 19th IUPAP International Conference on Statistical Physics, Xiamen, China, August 1995.

5. A. J. Haslam, S. C. McGrother, G. Jackson, A. G. Vanakaras and D. J. Photinos, *Computer simulation of rod-plate mixtures*, 6th EC Network meeting on Molecular Organisation in Liquid Crystals resulting from Particular Intermolecular Interactions, St. Pierre de Chartreuse, France, September 1997.

6. A. J. Haslam, S. R. Phillpot, D. Wolf and D. Moldovan, *Role of grain rotation in grain growth*, Materials Research Society Fall Meeting, Boston, Massachusetts, USA, November 2000.

7. D. Moldovan, D. Wolf, S. R. Phillpot and A. J. Haslam, *Atomistic and mesoscopic simulation of grain growth in nanocrystalline thin films*. USACM: Sixth US National Congress on Computational Mechanics, Dearborn, Michigan, USA, 1 – 4 August, 2001.

8. D. Moldovan, D. Wolf, S. R. Phillpot and A. J. Haslam, *Multiscale Simulation of Grain Growth in Nanocrystalline Thin Films*, workshop *Multiscale Modeling, Simulation and Visualization and Their Potential for Future Aerospace Systems*, NASA Langley Research Center, Hampton, VA, USA, 5 – 6 March 2002.

9. D. Moldovan, D. Wolf, S. R. Phillpot and A. J. Haslam, *Combined atomistic and mesoscale simulation of microstructural evolution in polycrystalline materials*, Materials Research Society Spring Meeting, San Francisco, California, USA, 2 – 5 April 2002.

10. D. Wolf, D. Moldovan, S. R. Phillpot, and A. J. Haslam, *Grain growth in nanocrystalline thin films: a case study for multiscale simulation of microstructural evolution in polycrystalline materials* (invited talk), International Conference on Multiscale Materials Modelling, Queen Mary, University of London, UK, June 2002.

11. M. A. Franco-Melgar, A. J. Haslam, S. Varga, and G. Jackson, *Ordering and fluid phase equilibria in systems of chain molecules*, 16*th* European Conference on Thermophysical Properties, London, UK, 3 September 2002.

12. M. A. Franco-Melgar, A.J. Haslam, S. Varga, and G. Jackson, *Ordering and fluid phase equilibria in systems of cylindrically symmetrical molecules*, 32nd Winter Meeting on Statistical Physics, Taxco, México, 8 January 2003.

13. M. Franco-Melgar, A. J. Haslam, and G. Jackson, *An analytical Onsager-like equation of state of ordering transitions in systems of attracting rod-like particles* (poster), 18*th* Thermodynamics Conference, Thermodynamics 2003, Cambridge, UK, 9 April 2003.

14. A. J. Haslam and C. S. Adjiman, *Simulation of entangled polyethylene melts by the method of Padding and Briels*, 3rd EU consortium meeting on Polymer Modelling at Integrated Length Scales, Thessaloniki, Greece, May 2003.

15. A. J. Haslam, V. Yamakov, D. Moldovan, D. Wolf, S. R. Phillpot and H. Gleiter, *Effect of grain growth on grain-boundary diffusion creep in Nanocrystalline Pd by molecular-dynamics simulation*, Materials Research Society Fall Meeting, Boston, Massachusetts, USA, December 2003.

16. M. A. Franco-Melgar, A. J. Haslam, and G. Jackson, *Ordering and fluid-phase equilibria in systems of liquid crystals* (poster), Foundations of Molecular Modeling and Simulation (FOMMS) 2003, Keystone, Colorado, USA, 9 July 2003.

17. M. A. Franco-Melgar, A. J. Haslam, and G. Jackson, *Fluid-phase equilibria and ordering transitions in systems of complex fluids through a statistical-mechanics based analytical equation of state*, British Liquid Crystal Society (BLCS) Annual Meeting, Manchester, UK, 6 April 2004.

18. D. Wolf, V. Yamakov, A. J. Haslam, S. R. Phillpot, H. Gleiter and A. Mukherjee, *'Microstructure and Deformation Physics' of Nanostructured Materials*, USACM Workshop on Computational Nanomechanics of Materials, Chicago, USA, 26 – 27 April 2004.

19. A. J. Haslam, V. Yamakov, D. Moldovan, D. Wolf, S.R. Phillpot and H. Gleiter, *Stress-enhanced grain growth in nanocrystalline materials* (invited talk), Special Symposium *Modeling and Simulation Materials Nanoworld* at 3rd International Conference *Computational Modeling and Simulation of Materials*, Acireale, Sicily, Italy, 30 May – 4 June, 2004; published as Vol. 44 *Advances in Science and Technology*, 2004, p285.

20. A. J. Haslam, V. Yamakov, D. Moldovan, D. Wolf, S. R. Phillpot and H. Gleiter, *Stress-Enhanced Grain Growth in Nanocrystalline Materials by Molecular-Dynamics Simulation* (invited seminar), Argonne National Laboratory, Argonne, Illinois, USA, 26 June 2004.

21. A. J. Haslam, V. Yamakov, D. Moldovan, R. Ding, D. Wolf, and S. R. Phillpot, *Multiscale simulation of static and dynamic grain growth in polycrystalline thin films*, 2nd Multiscale Modeling Conference, UCLA, Los Angeles, California, USA, 11–15 October, 2004.

22. M. A. Franco-Melgar, A. J. Haslam, and G. Jackson, *Maier-Saupe Theory: the Onsager Trial Function Approach*, 33rd Topical Meeting on Liquid Crystals of the German Liquid Crystal Society (33 Arbeitstagung Flüssigkristalle), Paderborn, Germany, 16 March 2005.

23. D. Wolf, A. J. Haslam, V. Yamakov, D. Moldovan, R. Ding and S. R. Phillpot, *Interplay between High-temperature Deformation and Grain Growth in Nanocrystalline Materials by Hierarchical Multiscale Simulation*, 2005 Materials Research Society Spring Meeting, San Francisco, California, USA, 28 March – 1 April, 2005.

24. A. J. Haslam, C. S. Adjiman, A. Galindo, G. Jackson and P. Paricaud, *Predicting enhanced absorption of gases in polyethylene using SAFT-VR*, 19th Thermodynamics Conference, Thermodynamics 2005, Sesimbra, Portugal, 5 – 8 April 2005.

25. N. von Solms, A. J. Haslam, P. Paricaud, C. S. Adjiman, A. Galindo, G. Jackson, M. L. Michelsen, and G. M. Kontogeorgis *Phase equilibrium in the polyethylene manufacturing process - a Comparison of PC-SAFT and SAFT-VR approaches*, 19th Thermodynamics Conference, Thermodynamics 2005, Sesimbra, Portugal, 5 – 8 April 2005.

26. M. A. Franco-Melgar, A. J. Haslam, and G. Jackson, *Analytical equation of state for liquid crystals and mixtures* (poster), 1st Conference on the Glass and Amorphous State (GLAMOR 2005), Cambridge, UK, 12 April 2005.

27. A. J. Haslam and C. S. Adjiman, *Mesoscale simulation of entangled polyethylene melts*, 7th EU consortium meeting on Polymer Modelling at Integrated Length Scales, El Saler, Spain, 14–15 April 2005

28. A. J. Haslam, C. S. Adjiman, A. Galindo and G. Jackson, *Gas absorption in polyethylene using SAFT-VR*, 7th EU consortium meeting on Polymer Modelling at Integrated Length Scales, El Saler, Spain, 14–15 April 2005

29. A. J. Haslam, A. Galindo and G. Jackson, *Thermodynamic modelling of hydrates*, Quarterly Meeting of Department of Trade and Industry project *Integrated Sensors, modelling and control for oilfield fluids and processes*, Imperial College London, UK, 19 September 2005.

30. A. J. Haslam, C. S. Adjiman, G. Jackson and A. Galindo, *Predicting enhanced absorption of gases in polythene using SAFT-VR* (poster), CPSE Industrial Consortium Autumn Meeting, Imperial College London, UK, 29 September 2005

31. B. P. Ló, A. J. Haslam and C. S. Adjiman, *Parameter estimation for stochastic differential equation model: algorithm and application to a model of polymer rheology*, CPSE Industrial Consortium Autumn Meeting, Imperial College London, UK, 29 September 2005

32. B. P. Ló, A. J. Haslam and C. S. Adjiman, *Parameter estimation for stochastic differential equations: algorithm and application to polymer melt rheology*, American Institute of Chemical Engineering Annual Meeting, Cincinatti, Ohio, USA, 30 October – 4 November 2005

33. A. J. Haslam, A. Galindo and G. Jackson, *Progress in the modelling of hydrates*, Quarterly Meetings of Department of Trade and Industry project *Integrated Sensors, modelling and control for oilfield fluids and processes*: Process Systems Enterprises, Hammersmith, London, UK, 19 December 2005; Schlumberger Cambridge Research, Cambridge, UK, 20 March 2006; Imperial College London, UK, 19 June 2006.

34. A. J. Haslam, *Idiots guide to molecular-dynamics simulation*, Mini Symposium on Molecular Simulation, Centre for Process Systems Engineering, Imperial College London, UK, 28 April 2006

35. A. J. Haslam, *Crystals and Defects*, Mini Symposium on Molecular Simulation, Centre for Process Systems Engineering, Imperial College London, UK, 28 April 2006

36. A. J. Haslam, *Dynamic grain growth in fcc metal by molecular dynamics simulation*, Imperial College Simulation Meeting, Centre for Process Systems Engineering, Imperial College London, UK, 28 April 2006

37. A. J. Haslam, A. Galindo and G. Jackson, *"Warm ice and antifreeze": Improving hydrate modelling with SAFT-VR* (poster), CPSE Poster Day, Centre for Process Systems Engineering, Imperial College London, 30 June 2006.

38. A. J. Haslam, A. Galindo and G. Jackson, *"Warm ice and antifreeze": Improving hydrate modelling with SAFT-VR*, Mini Symposium on Statistical Mechanics and Simulation, Centre for Process Systems Engineering, Imperial College London, UK 11 July 2006.

39. J. Deschamps, M.A. Franco-Melgar, A. J. Haslam, J. P. M. Trusler and G. Jackson, *Developing generalised Onsager models with Maier-Saupe interactions from experimental saturation pressure and density data* (poster), International School of Liquid Crystals, 13th Workshop: *Colloids, Interfaces and Liquid Crystals*, Erice, Sicily, 19–25 July 2006.

40. A. J. Haslam, Amparo Galindo, George Jackson, Julio Jover, Erich Müller and Stephen Richardson, *Modelling Asphaltenes using SAFT or related approaches*, Crude Oil Fouling Meetings, part of 14th and 15th IHS ESDU Oil Industry Fouling Working Party Meetings: Imperial College, London, UK, 27 March, 2007; Imperial College, London, UK, 25 September, 2007.

41. A. J. Haslam, S. Dufal, A. Galindo and G. Jackson (poster), *Modelling gas clathrate hydrates: incorporating an advanced thermodynamic description of the fluid*, Eleventh International Conference on Properties and Phase Equilibria (PPEPPD 2007), Hersonissos, Crete, Greece, May 20–25, 2007

42. A.J. Haslam, A. Galindo and G. Jackson, *Predicting binary-interaction parameters for use in molecular-based equati ons of state* (poster), 20th Thermodynamics Conference, Thermodynamics 2007, Rueil Malmaison, Paris, France, 26–28 September 2007.

43. A. J. Haslam, A. Galindo and G. Jackson, *Predicting binary-interaction parameters for use in molecular-based equations of state*, 23rd European Symposium on Applied Thermodynamics (ESAT), Lyons France, 29th May–1st June 2008.

44. M. A. Franco-Melgar, A. J. Haslam, and G. Jackson, *Algebraic description of nematic order in attracting rod-like particles and the Maier-Saupe model of liquid crystals using the Onsager trial-function approach* (poster), 7th Liquid Matter Conference, Lund, Sweden, 27th June – 1st July 2008.

45. A. J. Haslam, A. Galindo, G. Jackson, J. Jover, E. A. Müller and S. Richardson, *Thermodynamic modelling of asphaltene-oil systems using SAFT*, Crude Oil Fouling Meetings, part of 17th and 18th IHS ESDU Oil Industry Fouling Working Party Meetings: IHS ESDU, Bracknell, UK, 8–11 April, 2008; Imperial College, London, UK, 23–26 September 2008

46. A. J. Haslam, A. Galindo and G. Jackson, *Predicting binary-interaction parameters for use in modelling fluid mixtures*, AIChE Fall Meeting, Pennsylvania Convention Center, Philadelphia, PA, USA, November 16–21, 2008.

47. A. J. Haslam, *Defects – the link between crystallisation and perfect crystals*, Workshop – *Predicting and Controlling Crystallisation*, Dept. of Chemical Engineering, Imperial College London, UK, 5–6 February 2009.

48. A.J. Haslam, A. Galindo and G. Jackson, *Thermodynamic modelling of hydrate phase equilibria with SAFT-VR*, Final Meeting of Department of Trade and Industry project *Integrated Sensors, modelling and control for oilfield fluids and processes*: Process Systems Enterprises, Hammersmith, London, UK, 19 March 2009.

49. S. Dufal, A. J. Haslam, A. Galindo, G. Jackson, and E. Boek, *Modelling gas clathrate hydrates using SAFT-VR* (poster), 11*th* International Conference on Petroleum Phase Behavior and Fouling Petrophase Conference (PETROPHASE2010), Jersey City, USA, 13-17 June 2010.

50. H. Domínguez, A. J. Haslam, G. Jackson, and E. A. Muller, *Computer simulations of the liquid-liquid and liquid-vapor coexistence curves for the perfluorohexane + n-heptane system* (poster), 8*th* Liblice Conference on Statistical Mechanics of Liquids, Hotel Myslivna, Brno, Czech Republic, 15 June 2010.

51. S. Dufal, A. J. Haslam, A. Galindo, G. Jackson, and E. Boek, *Using SAFT-VR in modelling gas clathrate hydrates (poster), 20 Years of the SAFT Equation: Recent Advances and Challenges ($^{20}SAFT^{10}$)*, Universidad Autonoma de Barcelona/MATGAS, Bellaterra, Spain, 21 September 2010.

52. J. Jover, C. Nieto-Draghi, A. J. Haslam, A. Galindo, G. Jackson, and E. A. Müller, *Coarse-grained molecular simulations of asphaltene aggregation*, 12*th* International Conference on Petroleum Phase Behavior and Fouling Petrophase Conference (PETROPHASE2011), Imperial College London, 10-14 June 2011.

53. P.-A. Artola, A. Galindo, E. A. Müller, G. Jackson, and A. J. Haslam, *Understanding the phase behaviour of crude oil: asphaltene precipitation*, 12*th* International Conference on Petroleum Phase Behavior and Fouling Petrophase Conference (PETROPHASE2011), Imperial College London, 10-14 June 2011.

54. S. Dufal, A. J. Haslam, C. S. Adjiman, A. Galindo, and G. Jackson, *Modelling the phase-behavior of reservoir fluids: Study of alkanes-CO_2-water systems* (poster), 22*nd* Thermodynamics Conference, Thermodynamics 2011, Athens, Greece, 1 September 2011.

55. G. Jackson, P. E. Brumby, J. G. Sampayo, A. J. Haslam, A. Malijevsky, E. de Miguel, and E. A. Müller, *Complications with the use of mechanical expressions for the pressure tensor and interfacial tension in inhomogeneous systems* (poster), European Physical Society (EPS), 8*th* Liquid Matter Conference, Vienna, Austria, 8 September 2011.

56 R. Horton, M. Finnis, G. Jackson, A. Galindo, and A. J. Haslam, *An efficient method of calculating free energies of charged systems* (poster), European Physical Society (EPS), 8th Liquid Matter Conference, Vienna, Austria, 9 September 2011.

57. L. Wu, E. A. Müller, and G. Jackson, A. Galindo, and A. J. Haslam, *Generalised van der Waals-Onsager approach for attractive oblate cylinder particles* (poster), European Physical Society (EPS), 8*th* Liquid Matter Conference, Vienna, Austria, 9 September 2011.

58. P.-A. Artola, A. Georgiadis, A. Galindo, E. A. Müller, G. Jackson, and A. J. Haslam, *Describing the phase behaviour of crude oil: PT diagrams and asphaltene precipitation* (poster), International SAFT2011 Discussion Meeting on the Thermodynamic Modelling Crude Oil, Scientific & Technical Center of TOTAL Exploration-Production, Pau, France, 24–25 October 2011.

59. S. Dufal, A. J. Haslam, A. Galindo, and G. Jackson, *Modelling gas clathrate hydrates with SAFT-VR* (poster), International SAFT2011 Discussion Meeting on the Thermodynamic Modelling Crude Oil, Scientific & Technical Center of TOTAL Exploration-Production, Pau, France, 24–25 October 2011.

60. A. J. Haslam, *Modelling hydrate phase equilibria: van der Waals and Platteeuw theory*, International SAFT2011 Discussion Meeting on the Thermodynamic Modelling Crude Oil, Scientific & Technical Center of TOTAL Exploration-Production, Pau, France, 24–25October 2011.

61. R. Horton, M. Finnis, G. Jackson, A. Galindo, and A. J. Haslam, *Towards an Efficient Method of Calculating Free Energies of Charged Systems*, CECAM Workshop – Free energy calculations: From theory to applications, Ecole des Ponts, Champs-sur-Marne, France, 6 June 2012.

62. S. Dufal, A. J. Haslam, G. Jackson, and A. Galindo, *Modelling the phase equilibria of CO_2-brine systems*, 26th European Seminar on Applied Thermodynamics (ESAT), Potsdam, Germany, 8 October 2012.

63. R. M. Horton, A. J. Haslam, A. Galindo, G. Jackson, and M. Finnis, *A novel methodology for the description of the free-energetic contribution of charged defects in solid electrolytes*, Deutsche Physikalische Gesellschaft (DPG) Spring Meeting, Regensburg, Germany, 10–15 March 2013.

64. S. Dufal, A. J. Haslam, T. Lafitte, A. Galindo and G. Jackson, *Developing an accurate generic description of association interactions in fluids of molecules formed from Mie segments within the Wertheim TPT1 approach* (poster), 13th International Conference on Properties and Phase Equilibria for Product and Process Design (PPEPPD) 2013, Iguazu Falls, Argentina-Brazil, 26 - 30 May 2013.

65. S. Dufal, A. J. Haslam, T. Lafitte, A. Galindo, and G. Jackson, *The A in SAFT: investigating the association contributions within a Wertheim TPT1 treatment*, 13th International Conference on Properties and Phase Equilibria for Product and Process Design (PPEPPD) 2013, Iguazu Falls, Argentina-Brazil, 26-30 May 2013.

66. O. A. Oyewunmi, A. I. Taleb, A. J. Haslam, and C. N. Markides, *An Assessment of Working-Fluid Mixtures using SAFT-VR Mie for Use in Organic Rankine Cycle Systems for Waste-Heat Recovery*, 13th UK Heat Transfer Conference, Imperial College London, 2–3 September 2013.

67. S. Z. Al Ghafri, A. Galindo, A. Georgiadis, A. J. Haslam, G. Jackson, G. C. Maitland, and J. P. M. Trusler, *Phase behaviour of mixtures containing carbon dioxide with heptane and methylbenzene: a comparison of experiment with SAFT-γ-Mie predictions*, 23rd Thermodynamics Conference, Thermodynamics 2013, Manchester, 3 - 6 September 2013.

68. S. Dufal, A. J. Haslam, T. Lafitte, A. Galindo, and G. Jackson, *The Wertheim TPT1 approach applied to the association of Mie segments* (poster and short oral presentation), 23rd Thermodynamics Conference, Thermodynamics 2013, Manchester, 3 - 6 September 2013.

69. D. K. Eriksen, S. Dufal, A. Galindo, A. J. Haslam, and George Jackson, *A physically rigorous procedure for the development of ion-model parameters for use in molecular-based electrolyte equations of state* (poster), 23rd Thermodynamics Conference, Thermodynamics 2013, Manchester, 3 - 6 September 2013.

70. O. A. Oyewunmi, A. I. Taleb, A. J. Haslam, and C. N. Markides, *An Assessment of Working-Fluid Mixtures in Organic Rankine Cycles for Waste-Heat Recovery using SAFT-VR*, ASME ORC 2013, 2nd International Seminar on ORC Power Systems, De Doelen, Rotterdam, The Netherlands, 7–8 October 2013.

71. S. Dufal, J. Schreckenberg, C. S. Adjiman, A. J. Haslam, G. Jackson, and A. Galindo, *Modelling electrolyte solutions using the SAFT-VRE Mie equation of state* (poster), American Institute of Chemical Engineers (AIChE), 2013 Annual Meeting, San Francisco, USA, 3 - 8 November 2013.

72. O. A. Oyewunmi, A. I. Taleb, A. J. Haslam, and C. N. Markides, *The use of SAFT-VR Mie in the assessment of working-fluid Mixtures for use in Organic Rankine Cycles for waste-heat recovery*, SAFT 2014 – "from SAFT to Experiment and Back", Tróia, Portugal, 22–24 April, 2014.

73. S. Dufal, A. J. Haslam, T. Lafitte, A. Galindo, and G. Jackson, *The A in SAFT: investigating the association contributions within a Wertheim TPT1 treatment*, SAFT 2014 – "from SAFT to Experiment and Back", Tróia, Portugal, 22–24 April, 2014.

74. S. Z. Al Ghafri, A. Georgiadis, A. Galindo, A. J. Haslam, C. S. Adjiman, V. Papaioannou, G. Jackson, G. C. Maitland, and J. P. M. Trusler, *Phase behaviour of the system (carbon dioxide + n-heptane + methylbenzene) and (carbon dioxide + methane + methylbenzene): a comparison between experimental data and SAFT-γ Mie predictions*, SAFT 2014 – "from SAFT to Experiment and Back", Tróia, Portugal, 22–24 April, 2014.

75. D. K. Eriksen, S. Dufal, A. J. Haslam, A. Galindo and G. Jackson, *Intermolecular potential model development for ionic species with the SAFT-VRE Mie approach*, SAFT 2014 – "from SAFT to Experiment and Back", Tróia, Portugal, 22–24 April, 2014.

76. A. J. Haslam, S. Z. Al Ghafri, A. Georgiadis, A. Galindo, C. S. Adjiman, V. Papaioannou, G. Jackson, G. C. Maitland, and J. P. M. Trusler, *Experimental and modelling study of the phase behaviour of (CO2 + synthetic crude oil) and related mixtures* (poster), Petrophase XV, San Luis Resort Spa and Conference Center, Galveston, TX, USA, June 8–12 2014.

77. P. E. Brumby, H. H. Wensink, A. J. Haslam and G. Jackson, *Structure and interfacial tension of a hard-rod fluid in planar confinement*, Ninth Liblice Conference on the Statistical Mechanics of Liquids, Sec Dam Lake, Czech Republic, 15–20 June 2014.

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RESEARCH

I am currently a member of the Molecular Systems Engineering group (MSE) group in the Department of Chemical Engineering at Imperial College. I have been engaged in several different avenues of research, alongside several members of the academic staff within the department, including Prof. Claire Adjiman, Prof. Amparo Galindo, Prof. George Jackson, Prof. Martin Trusler, Prof. Erich Müller and, most recently, Dr. Christos Markides.

INDUSTRIALLY DRIVEN / APPLIED RESEARCH

Qatar Carbonates and Carbon Storage Research Centre (QCCSRC)

Since the autumn of 2009, my employment at Imperial College London has been as a member of the QCCSRC, which is a multifaceted research centre aimed principally at furthering understanding of all aspects of carbon sequestration in saline aquifers, as well as issues relating to Qatari oil and gas. An aquifer is an underground layer of water-bearing permeable rock; the name of the centre reflects the carbonate nature of the rock comprising the Qatari aquifers. My role has been to direct and coordinate the research in our group relating to the thermodynamics of all the relevant fluids – principally hydrocarbons, carbon dioxide, water and brines. In association with PhD students Simon Dufal and, latterly, Daniel Eriksen, this has involved the development of new models for use with the latest in-house version of the statistical associating fluid theory, SAFT-VR Mie, as well as a refinement of our electrolyte-modelling capability, SAFT-VRE Mie. Most recently, the focus of the research lies on a tractable implementation of the square-gradient theory to calculate interfacial tensions, in conjunction with our SAFT approaches.

Asphaltene – oil systems

One of my principal research responsibilities lies in the area of thermodynamic modelling of *asphaltenes* and their phase equilibria in crude oils, which constitute an increasingly topical problem in the oil industry. The problem of crude-oil fouling, wherein asphaltenic deposits block pipes at various points during the recovery of crude oil, represents an enormous financial burden in the oil industry, but yet is still not fully understood. We recognise the deposition of asphaltene as a thermodynamic phase-equilibrium phenomenon, whereby the successful prediction of asphaltene deposition rests on the appropriate choice of underlying molecular models to represent the asphaltene and the oil. Since the molecular nature of ashphaltenes remains the subject of heated controversy, this constitutes a considerable challenge. To date, my

most-successful modelling has resulted from drawing an analogy between oil-asphaltene and alkane-polystyrene phase equilibria, the latter being a much-more-clearly characterised system.

Organic Rankine cycles – conversion of waste heat to useful energy

Following the development in our research group of the state-of-the-art, molecular-based equation of state (EoS) SAFT-VR Mie, using a single model we are now able to routinely capture a wider variety of thermodynamic properties of a fluid with quantitative accuracy; among these are calorific quantities and second-derivative properties such as heat capacities. This has provided the opportunity to embark on research into the design of working fluids for heat engines based on Rankine and related cycles. These organic Rankine cycle (ORC) devices can be used to convert different sources of heat, including waste heat, to useful energy. Their analysis requires quantitative accuracy in the prediction of the calorific quantities that are used to compute efficiencies; hitherto it had not been possible to supply this information (at the required quality) cheaply using an EoS. In this context, I have embarked on a collaboration with Dr Christos Markides (of Imperial College London), who is an expert in the design and analysis of these types of engine.

Gas (clathrate) hydrates

Also related to the theme of *flow assurance*, I have a strong interest in the study of *gas (clathrate) hydrates*. The plugging of pipelines by this unfamiliar form of "ice" remains a topic of enormous importance in the recovery of natural gas from deep-sea reserves. Between 2005 and 2009 I was involved in a programme concerning thermodynamic modelling of gas hydrates, working in collaboration with other colleagues at Imperial College (led by Prof Martin Trusler), Schlumberger Cambridge Research (SCR) and Process Systems Enterprises plc (PSE). My research centred on the development of hydrate and related thermodynamic modelling tools for incorporation in flow simulations for gas risers. An important aspect of this work was the thermodynamic modelling of aqueous mixtures involving natural gases and hydrate inhibitors, such as methanol. As part of this work, I was involved, with Dr Mike Williams of Schlumberger, in the incorporation of our thermodynamic equation of state (SAFT-VR) into their *Eclipse* reservoir simulator. I was also involved, with Prof Costas Pantelides and Dr Praveen Lawrence of PSE, in the incorporation of a thermodynamic hydrate modelling tool in the *gPROMS* process simulator.

Gas-polymer systems

In a recent collaboration with Borealis, an international plastics-manufacturing company, I carried out a thermodynamic study of *gas absorption in polyethylene* (PE) with a view to improving the efficiency of PE manufacture in the gas-phase polymerisation process. The result of this study, which was published as a book chapter (see *Publications*), was a 30%

improvement in yield of PE in bench reactor experiments. This work is featured as a *Research Highlight* later in this document.

FUNDAMENTAL RESEARCH

Intermolecular forces

At the heart of modelling fluids, whether by molecular simulation or statistical-thermodynamic theory, is the potential model that underlies the representation of intermolecular forces. In mixtures of two or more different components, the intermolecular potential for the interaction of unlike molecules is generally assumed to be given by averages of those of the like-like interactions: an arithmetic mean for the size parameter (the Lorentz rule); a geometric mean for the energy parameter (the Berthelot rule). When using these rules, failure to adequately model a mixture is frequently regarded as a failure of the theory; the potential is implicitly assumed to be (at least approximately) correct. This belief stems from the successful use of the Lorentz-Berthelot (LB) rules over many years, albeit for the analysis of systems of simple molecules. The theoretical origins of the LB rules can be traced back to the seminal works of London in the early 20th century, which represent the dispersion interaction of simple molecules. By pursuing an analogous treatment, but starting with more-complicated interactions (*e.g.*, incorporating polar in addition to dispersion interactions) I have shown that, theoretically, the LB rules are expected to provide a poor representation for mixtures including polar or, in particular, hydrogen-bonding fluids; similarly mixtures involving large molecular-size asymmetry are expected to be poorly represented using the LB rules. Since mixtures incorporating polar molecules or involving size asymmetry are common in problems of current industrial interest, this work has already proven to be of great value throughout other areas of my research; most recently it has made an important contribution in respect of providing a means to assign parameter values in our electrolyte modeling tool, SAFT-VRE Mie, thereby reducing the number of adjustable parameters and helping to minimize parameter degeneracy.

In June 2014, I was highly commended by the Department of Chemical Engineering for my "outstanding contribution in research"; part of the assessment for this award was based on my paper, *Prediction of binary intermolecular potential parameters for use in modelling fluid mixtures* (Fluid Phase Equilibria, 2008), in which my work on intermolecular forces is detailed. I was presented with an award in recognition of this commendation at the inaugural Postdoctoral Symposium; only five post-doctoral researchers from a total of 80 working in the Department were similarly recognized.

Polymers

Polymers represent a recurring theme in my research, beginning with the Monte Carlo simulation studies of simple "pearl-necklace" polymers that I carried out during my Ph.D.. I am currently involved in related research, with Julio Jover and Erich Müller, in studies of mixtures chains of this type with large spheres, which can be thought of as representing colloids or asphaltenes. I have also been active in multiscale dynamic simulation of more-realistic polymers. Information drawn from molecular-dynamics (*atomistic*) simulation was used to provide coarse-grained information and parameterise a coarse-grained model in *mesoscale* dynamic simulations. Ultimately, the goal of this type of research will be to provide information for a further coarse-graining to the *macroscale* simulation of polymer melt rheology, such as that in which I have been involved with Bernardino Lo, a graduate student with Dr. Claire Adjiman. This hierarchical approach to *multiscale modelling* is also a recurrent theme in my research, and underpinned my research into the manner in which defects affect the physical properties of metals.

Liquid Crystals

My first involvement in liquid-crystal research, at the University of Patras in Greece, concerned the development of a Monte Carlo simulation code to simulate mixtures of rod-like molecules (which individually form nematic liquid crystals) and plate-like molecules (which individually form discotics) in search of evidence of a so-called *biaxial nematic* liquid-crystal phase. Since coming to London in 2001, an ongoing area of my research has been the statistical-thermodynamic modelling of nematic liquid crystals with a view to obtaining an engineering equation of state capable of predicting the phase equilibria of this interesting and important class of compounds. This work subsequently became the focus of the Ph.D. studies of Mario Franco-Melgar who, although not directly under my supervision, generously acknowledged me in his thesis as his "other supervisor".

Solids: metallic polycrystals and the role of defects

All of the above research areas may loosely be cast under the heading *fluids*; half of research output relates to this broad area. The remaining half is concerned with my interest in the role played by *defects*, particularly *grain boundaries*, in the physical characteristics of metals. This work was the focus of my research at the Argonne National Laboratory in the USA, both as a Research Associate and later, during a leave-of-absence from Imperial College, as a Visiting Scientist. Under the leadership of Dr. Dieter Wolf, I worked as part of a team studying grain growth and deformation in metals using a hierarchical approach to multiscale simulation, similar to that described earlier in the context of polymer dynamics. One of the studies I carried out is featured as a *Research Highlight* later in this document. Since coming to London in 2001 I have maintained my interest in this field. I delivered an invited talk on the subject of stress-enhanced

grain growth at a major international conference in 2004; it was to investigate novel ideas that I had proposed in this area that I was invited to return to Argonne National Laboratory as a Visiting Scientist that same year.

TEACHING

Although my appointments thus far have all been specifically research appointments, I have taken a number of teaching roles when opportunities arose. My view is that, within universities, teaching is of at least equal, if not higher importance than research; I believe that this is also the majority view outside academia. Based on my experience so far, while undoubtedly hard and challenging work, I have found teaching to be highly rewarding and, moreover, frequently great *fun*.

Class tutorials: Thermodynamics

For the past ten years (and continuing this year) I have taught thermodynamics in class tutorials to first-year chemical engineering students at Imperial College; formally this involves two hours per week through the first two terms and into the early weeks of term three (informally, it involves considerably more in terms, for example, of e-mail communications to answer students' questions). The tutorials supplement the students' lectures and are primarily problem-based. I have been told throughout that the students enjoy my teaching and rate it highly. Over recent years formal assessment has been provided in terms of the Student On-Line Evaluations (SOLE), in which I have consistently scored very highly; students' (anonymous) comments have been universally positive – I quote a selection here: "*Excellent Tutoring*"; "*I look forward to his tutorials enthusiastically*"; "*A few tutors should definitely learn from him*"; "*Most helpful academic tutor thus far*"; "*Wonderful, I love how he passes on his enthusiasm!*"; "*Top quality tutoring. Explains things thoroughly and clearly*". In 2014 I was nominated by my students in the newly established Student Academic Choice awards in the *Best Tutor* category, and was awarded a commemorative mug in recognition of this.

Technical Presentations Workshops

From 2009 to 2013 I was responsible for the *Technical Presentations* workshops (formerly known as "Presentation Skills" workshops) undertaken by undergraduates as part of their Techno-Economic Project; initially this took place in the students' 3rd year, however in 2010 the project was transferred to the 2nd year, with both classes undertaking the project in the transition year. The purpose of these workshops is to give each undergraduate student an opportunity to give a technical presentation in a reasonably relaxed environment in which they can learn the basic ideas of good presentations; this allows them to make mistakes without serious consequence, providing a valuable learning opportunity. The year is divided into 12 groups of approximately a dozen students, divided into pairs. Each pair gives an oral presentation on a subject related to energy and the environment; the presentations have been prepared in advance

based on guidance that I provide. The presentations are assessed by two experienced graduate teaching assistants, as well as by the presenters' peers in the workshop, using assessment sheets that I designed; each workshop concludes with a group discussion on features of the presentations that went well, or that did not, common errors and so forth. My role is primarily an organizational one, although I do actively take part in some of the workshops. The structure of the workshops is of my devising – prior to my involvement, the workshops were rather *ad hoc*, with the result that they were not taken very seriously by the students. I contact all of the students in advance of the workshops, requiring each pair to choose and register a title from a list of topics that I provide; I then coordinate each workshop to avoid undue repetition of the same titles, furnishing printed schedules; together with the assessment sheets, this gives the sense that the Department takes the workshops seriously so that, in turn, the students do also.

Lectures: Statistical Thermodynamics, and Molecular Simulation

Over recent years, I have developed a graduate-level course entitled *An Introduction to Statistical Thermodynamics and its Application in Equation-of-State Modelling of Fluids*, which I give on an annual or twice annual basis to new students arriving in our research group. The purpose of this course is to provide the background theory that is implicit in most of the research conducted in our group. In particular, I illustrate the development of the Statistical Associating Fluid Theory (SAFT), and set this in context with other more-traditional equations of state. The course comprises approximately 14 hours of lectures, and is accompanied by a detailed set of printed notes that I have prepared and continue to augment (an electronic copy of these notes is available on request). Recently, I also gave this course to interested members of the Qatar Carbonates and Carbon Storage Research Centre (QCCSRC) at Imperial College, when it was attended by about 15 participants locally, as well as by two participants from *Shell*, who sponsor the Centre, via video-conference link. Feedback received about this course has been very positive.

On an occasional basis, I have also lectured to our graduate students as a group on the basics of Molecular Simulation.

Other teaching activities

When the new undergraduate teaching laboratories were established in the Chemical Engineering Department at Imperial College in 2011, I developed scripts for three of the experiments, which I understand to have been very well received by the students.

During my Ph.D. studies at the University of Sheffield I taught in the first-year undergraduate Physical Chemistry Laboratory for two years. Laboratory classes were supervised by a member of the academic teaching staff, together with two post-graduate demonstrators who were expected to be familiar with *all* the experiments and the scientific principles involved.

Although our teaching was not formally rated, my verbal feedback from the students was entirely positive. Not all demonstrators were invited to continue beyond their first year in the teaching laboratory; that my teaching was valued by the department was testified by my being invited to continue teaching for a second year. As a further testament, during my Ph.D. studentship the Department of Chemistry selected me as the person to whom they directed outside enquiries from parents seeking graduate tutors for their children studying for 'A' Level examinations; I undertook such tuition with several students. Since I was in some sense representing the Department in this role, I infer that they had great confidence in my teaching ability. I mention here also that during my Ph.D. studies at the University of Sheffield I conducted class tutorials in Physical Chemistry as a substitute for my supervisor when he was absent.

Lectures: Physical Chemistry; Molecular Simulation

Although having never been employed in a lecturing capacity, I do have some experience of lecturing to undergraduates. During periods of absence from the University, my Ph.D. supervisor, George Jackson, occasionally called upon me to substitute for him in lectures, both in his core second-year class in Physical Chemistry (ca 100 – 150 students) and elective third-year class in Molecular Simulation (ca 30 – 40 students). Although to date he has supervised upwards of 30 Ph.D. students, at least three of whom have gone on to senior academic appointments, Prof. Jackson has never, as far as I am aware, asked any other of his graduate students to lecture in his place. I infer from this that he rated my lecturing abilities very highly.

Supervision and guidance of research students

I have been co-supervisor to three PhD students – Simon Dufal (successfully defended, 2013), Robert Horton (successfully defended, 2014) and Daniel Eriksen (ongoing) – as well as several Masters students. I take an active role in supervision of final-year undergraduate projects; I supervise the Undergraduate Research Opportunities Programme (UROP) projects in our research group (nine students over recent summers).

In general, during my employment at Imperial College I have been asked to assist with the guidance of research students more than, perhaps, is usual for a Research Associate; this has been an enjoyable and rewarding part of my work and my performance in this regard is probably a principal reason for my promotion to Research Fellow in the summer of 2008. In addition to the students that I have co-supervised, I mention my close association with Mario Franco-Melgar (who currently holds a position in the Chemical Engineering Department at Monterrey, Mexico) and Bernardino Lo. I single out also for mention my close association with Gary Clark, working on the thermodynamic modelling of water; Gary graduated at the end of 2007 and went on to work in the group of Theresa Head-Gordon at the University of California, Berkeley. The Molecular Systems Engineering (MSE) group is relatively large, at any given time incorporating

typically a dozen graduate students, and I frequently interact also with many of these. It has become the custom for me to teach our incoming graduate students the rudiments of Linux / UNIX and of FORTRAN programming. Over time, I have become the "go-to" person for our students when they encounter problems in their work; recently, I have begun receiving similar requests for help from students outside the MSE group. These discussions with the students now account for a significant proportion of my time.

ADMINISTRATION AND PROFESSIONAL DEVELOPMENT

Organiser: Mini Symposium on *Molecular Simulation*, Centre for Process Systems Engineering, Imperial College London, UK, 28 April 2006.

Co-organiser: Mini Symposium on *Statistical Mechanics and Simulation*, Centre for Process Systems Engineering, Imperial College London, UK 11 July 2006.

Coordinator: Fluids Engineering Seminar Series 2008–2009, Dept. of Chemical Engineering, Imperial College London.

Co-organiser: Workshop – *Predicting and Controlling Crystallisation*, Dept. of Chemical Engineering, Imperial College London, UK, 5–6 February 2009.

Organiser: Workshop – *Thermodynamics at different scales: force-fields and methods*, Centre for Process Systems Engineering, Dept. of Chemical Engineering, Imperial College London, UK, 9–10 January 2014.

Acted as referee for articles in 17 different journals in chemical engineering and related disciplines, including the Journal of Chemical Physics, Molecular Physics, Industrial and Engineering Chemistry Research, Fluid Phase Equilibria, Macromolecules, and Energy and Fuels.

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RESEARCH HIGHLIGHT – THEORY:

In the industrial manufacture of polyethylene (PE) in gas-phase polymerisation reactors (GPRs), reacting alkenes are introduced in gaseous form, while the polymer produced forms a liquid phase, so that there is a vapour-liquid equilibrium (VLE) between the gases and (liquid) PE. The catalyst, at which the reaction takes place, resides in the PE-rich phase. Consequently, in order to maximise yield of polymer, it is essential to maximise the absorption of reacting alkenes in the PE (liquid) phase. Pressure is maintained in the reactor by the introduction of non-reacting diluent gases; nitrogen, the most common, is typically present in even larger quantities than the reacting alkenes.

Using SAFT-VR, a state-of-the-art version of the Statistical Associating Fluid Theory, I modelled VLE of gas + PE mixtures. I successfully reproduced available experimental binary-mixture data; it was evident from these calculations that absorption of gas in PE rises increasingly steeply at pressures approaching the saturation (vapour) pressure of the gas. Calculations for ternary mixtures (two gases + PE), for which experimental data are very scarce, suggested that less-volatile gases enhance absorption of more-volatile gases, while more-volatile gases inhibit absorption of less-volatile gases. If a similar effect is present in multi-component mixtures of many gases + PE, such as those used in the GPR process, then nitrogen, in particular, would act as an absorption inhibitor to reacting alkenes and its presence restrict the yield of polymer. My calculations for such mixtures suggested that indeed such an effect should be expected – and that by tailoring the mixture appropriately using, for example, pentane instead of nitrogen to pressurise the reactor, absorption of reacting alkenes may be approximately doubled, which would imply a large increase in yield.

Bench-reactor experiments, based on these calculations, were carried out recently by Borealis, our industrial partner. In these experiments diluent nitrogen was partially replaced by pentane. As predicted, this change in the non-reacting gases in the mixture resulted in an enormous increase in yield of polymer; the increase in polymerisation activity was 30%. This result could have a substantial impact in industrial polymerisation of polythene using the GPR process. It also casts light on the so-called co-monomer effect, in which increase in yield of polymer is observed in the GPR polymerisation of ethene in the presence of hexene co-monomer, since hexene is a less volatile gas than ethene.

This, and related work has been published in Fluid Phase Equilibria and forms a chapter of a book, *Multiscale Modelling of Polymer Properties*, published by Elsevier in 2006 (see *Publications*).

RESEARCH HIGHLIGHT – SIMULATION:

In the solid state metals are polycrystalline; rather than individual, large pieces of perfect crystal, metals consist of many tiny pieces of crystal, called grains, joined together in a sort of microscopic 3D "jigsaw puzzle." Grains are distinguished from one another by the different orientations of their crystal axes; the regions in which they meet constitute surface defects known as *grain boundaries*. In nature grains are not static, but grow, in so doing affecting the physical properties of the metal, making the process of grain growth one of great importance.

Using molecular dynamics (MD) I simulated a thin film of nanocrystalline palladium, a metal in which grain growth is rapid. Performing the calculations on a parallel computer enabled the simulation of a physically realisable, nanocrystalline microstructure of 25 grains with an average grain size of 15nm, containing almost 400,000 atoms for $\mathcal{O}(10)$ ns. I developed a suite of programs to visualise the evolving grain topology and to analyse features such as grain orientation and size.

The conventional picture of grain growth is that the process is driven by curvature-driven grain-boundary (GB) migration, reducing the total area of GBs in the material and so lowering the total excess energy. The simulations showed that in nanocrystalline materials grain rotations sometimes lead to the coalescence of neighbouring grains by eliminating the GB separating them, forming new, highly-elongated grains. Detailed analysis revealed that in grains neighbouring coalescence events, GB migration is accelerated, further enhancing the grain-growth process. These were invaluable insights, which have since been verified experimentally. These and other results from the MD simulations were used to parameterise our kinetic Monte Carlo (KMC) mesoscale simulation of grain growth, a type of finite-element simulation wherein the individual atoms are "thrown away" and the microstructure is modelled instead as linked sets of "nodes" mapping out the GBs and thus the grain topology. The KMC technique was developed to study much larger systems at far greater time scales, yet the simulations accurately reproduced the results of the MD simulations, confirming both our understanding of the underlying physics and the validity of the technique. More importantly, the simulations revealed that the competition between grain-boundary migration and grain rotation introduces a physical length scale, R_c, into the system, enabling the growth process to be characterized by two regimes. If the average grain size is smaller than R_c, as is the case in nanocrystalline materials, grain growth is dominated by the grain-rotation-coalescence mechanism. By contrast, if the average grain size is greater than R_c, then growth is dominated by curvature-driven grain-boundary migration. This is an outstanding example of successfully bridging length and time scales in simulation; moreover the "MD-to-mesoscale" scheme may be applied in any field in which multiple time and length scales are important.

Further details of this work may be found in Haslam *et al*, Mat. Sci. and Eng. A-Struct., 2001; Haslam *et al*, Comp. Mater. Sci., 2002 and Moldovan *et al*, Acta Mater., 2002 (see *Publications*).

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RELEVANT PERSONAL DETAILS

Full name: Andrew John Haslam Date of Birth: 15th October 1962 Marital Status: Single

EARLY EDUCATION

'A' levels:

- Chemistry (grade A), Physics (B), Mathematics (B) *1980*

'O' levels:

- Additional Mathematics (grade A) *1979*
- Mathematics (grade A), Chemistry (B), Physics (B), Biology (A), English literature (B), French (B) *1978*
- English language (B), Music ('O' level equivalent: gr. 5 theory & (piano) practical) *1977*

WORK EXPERIENCE (non-academic)

Hotel and restaurant work:

- Stow Lodge Hotel, Stow-on-the-Wold, Cheltenham, Glos., UK ..... *1984 – 1989*
  - Restaurant and bar work, latterly wine waiter and relief head waiter; calligrapher (menu writing etc).
- Restaurant Ship *Hispaniola*, Victoria Embankment, London, UK: pianist ..... *summer 1987*

Printing:

- Willow Press, Bourton-on-the-Water, Cheltenham, Glos., UK ..... *part time, 1988 – 1989*
  - Letterpress work, *e.g.*, type setting, machine operation (Heidelberg platen).

INTERESTS AND ACTIVITIES

Tennis:

- Winter-league team member, Moreton-in-Marsh Tennis Club, Glos., UK (*since 2010*);
  Team Captain, Sheffield University Tennis (*1990/1991 and summer 1994*);
  Captain, Sheffield University Tennis Club (*1992 – 1994*);
  Team Captain, Moreton-in-Marsh Tennis Club, Glos., UK (*1982 – 1989*).

Music:

- I love to play the piano; currently I am interested in the slow, easy-going music of the early part of the 20th Century. I also play classical and rag-time music.
- I love symphonic music, especially live.

Printing:

- From the early 1980s until going to the USA in 1998 I ran my own business as a self-financing hobby. This comprised small letterpress jobs including sub-contracted high-quality originals for lithographic reproduction, as well as calligraphy work, *e.g.*, wedding invitations, menus.

General:

- I love walking, and I regularly organise walks for members of the MSE group and their friends. Usually these are situated within Greater London, but two or three times per year I make it an outing to somewhere further afield, typically of historic interest.
- I read a lot for relaxation, mostly science-fiction and fantasy; I enjoy sci-fi on screen also.
- From my days in restaurant work, I have retained an interest in food and wine.
- In addition to my love of tennis, I am a keen follower and spectator of sport in general. While living in America I developed a passion for baseball, in particular the Chicago Cubs!