

# Yiannis N. Kaznessis

## Associate Professor

Department of Chemical Engineering and Materials Science, and Digital Technology Center,  
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Professor Kaznessis' research interests focus on computer modeling of biological matter, on the development of bioinformatics methods and on statistical mechanical modeling of biomolecular recognition phenomena. Professor Kaznessis teaches undergraduate "Chemical Engineering Thermodynamics", undergraduate "Process Dynamics and Control" and the graduate course "Statistical Thermodynamics and Kinetics". Professor Kaznessis is also the Director of the University of Minnesota Summer Bioinformatics Institute.

### Education

- Diploma, Chemical Engineering, Aristotle University of Thessaloniki, Greece, 1994.
- Ph.D., Chemical Engineering, University of Notre Dame, 2000.
- Postdoctoral Fellowship, University of Michigan and Pfizer Global Research and Development, 08/99-08/01

### Appointments

**ASSOCIATE PROFESSOR**, 08/01/07-

Department of Chemical Engineering and Materials Science, University of Minnesota  
Digital Technology Center, University of Minnesota

**ASSISTANT PROFESSOR**, 08/23/01-07/31/07

Department of Chemical Engineering and Materials Science, University of Minnesota  
Digital Technology Center, University of Minnesota

**DIRECTOR**, 01/01/03-present

University of Minnesota Summer Bioinformatics Institute

**POSTDOCTORAL FELLOW**, 08/99-08/01

Biomolecular Structure and Drug Design, Pfizer Global Research and Development.  
Department of Chemical Engineering, University of Michigan.

**RESEARCH ASSISTANT**, 09/94-08/99

Department of Chemical Engineering, University of Notre Dame, Ph.D. (2000).

**PROJECT MANAGER ASSISTANT**, 12/93-08/94

Euroconsultants S.A., Thessaloniki, Greece.

**RESEARCH ASSISTANT**, 01/91-05/92

Chemical Process Engineering Research Institute, Thessaloniki, Greece.

### Honors and Awards

- 2007 NSF CAREER
  - 2006 Fellow, Minnesota Supercomputing Institute
  - 2004 3M non-Tenured Faculty Award
  - 2003 IBM Young Faculty Award
  - 2003 Young Investigator Petroleum Research Fund Award
  - 2000 Postdoctoral Fellowship, University of Michigan/Pfizer GRD
  - 2000 SGI Computational Science and Visualization Award, University of Notre Dame
  - 1994 Fulbright Award
  - 1994, Technical Chamber of Greece Honor Award (1<sup>st</sup> in senior class)
  - 1991-1993, Greek National Fellowship Foundation Awards (IKY)
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## Research Publications

1. Y. N. Kaznessis, D. A. Hill, E. J. Maginn, "Molecular Dynamics Simulations of Polar Polymer Brushes", *Macromolecules*, Vol. 31, p. 3116, 1998.
  2. Y. N. Kaznessis, D. A. Hill, E. J. Maginn, "A Molecular Dynamics Study of Macromolecules in Good Solvents. Comparison with Dielectric Spectroscopy Experiments", *Journal of Chemical Physics*, Vol. 109, p. 5078, 1998.
  3. Y. N. Kaznessis, D. A. Hill, E. J. Maginn, "Dielectric Relaxation of Dipole-Inverted Macromolecules Using Computer Simulations", *Macromolecules*, Vol. 32, p. 6679, 1999.
  4. Y. N. Kaznessis, D. A. Hill, E. J. Maginn, "Concentration and Size Dependence of Dielectric Strength and Dielectric Relaxation of Flexible Polymers in Dilute and Semidilute Solutions of a Theta Solvent", *Macromolecules*, Vol. 32, p. 1284, 1999.
  5. Y. N. Kaznessis, D. A. Hill, E. J. Maginn, "Dielectric Relaxation of Concentrated Polymer Solutions via Molecular Dynamics Simulations", *Journal of Chemical Physics*, Vol. 111, p. 1325, 1999.
  6. Y. N. Kaznessis, L. Narashimhan, M. E. Snow, "Binding Free Energy Calculations for Benzamidine-Trypsin Complexes", *Proceedings of Foundations of Molecular Modeling and Simulation Conference, AIChE Symposium Series*, p. 283, 2000.
  7. Y. N. Kaznessis, M. E. Snow, C. J. Blankley, "Prediction of Blood-Brain Partitioning Using Monte-Carlo Simulations of Molecules in Water", *Journal of Computer-Aided Molecular Design*, Vol. 15, p. 697, 2001.
  8. Y. N. Kaznessis, S. Kim, R. G. Larson, "Simulations of Zwitterionic and Anionic Phospholipid Monolayers", *Biophysical Journal*, Vol. 82, p. 1731-42, 2002.
  9. Y. N. Kaznessis, S. Kim, R. G. Larson, "Specific Mode of Interaction Between Components of Model Pulmonary Surfactants Using Computer Simulations", *Journal of Molecular Biology*, Vol. 322, p. 569-582, 2002.
  10. L.M. Gordon, P.W. Mobley, W. Lee, S. Eskandari, Y. Kaznessis, M.A. Sherman, A.J. Waring, "Conformational mapping of the N-terminal peptide of HIV-1 GP41 in lipid detergent and aqueous environments using <sup>13</sup>C-enhanced Fourier transform infrared spectroscopy" *Protein Science*, Vol. 13, p. 1012-30, 2004.
  11. H. Wei, Y. Kaznessis, "Inferring gene regulatory relationships by combining target-target pattern recognition and regulator-specific motif examination" *Biotechnology and Bioengineering*, Vol. 89(1), p. 52-77, 2005.
  12. N. Ostberg, H. Khandelia, Y. Kaznessis, "Protegrin structure activity relationships: Using homology models of synthetic sequences to determine structural characteristics important for activity" *Peptides*, Vol. 26(2), p. 297-306, 2005.
  13. A. Langham, Y. Kaznessis, "Molecular dynamics simulations of the N-terminus of HIV GP-41 fusion peptide in SDS micelles" *Journal of Peptide Science*, Vol. 14(2), p. 316-328, 2005.
  14. S. Vicatos, V.B. Reddy, Y. Kaznessis, "Prediction of distant residue contacts with the use of evolutionary information" *Proteins, Bioinformatics, Structure and Genetics*, Vol. 58(4): 935-49, 2005.
  15. H. Salis, Y. Kaznessis, "Accurate Hybrid Stochastic Simulation of a System of Coupled Chemical or Biochemical Reactions", *Journal of Chemical Physics*, Vol. 122, p. 054103 1-13, 2005.
  16. H. Salis, Y. Kaznessis, "Numerical simulation of stochastic gene circuits" *Computers & Chemical Engineering*, Vol 29(3), p. 577-588, 2005.
  17. Y. Duan, V. Reddy, Y. Kaznessis, "Physicochemical and residue conservation calculations to improve the ranking of protein-protein docking solutions" *Protein Science*, Vol. 14(2), p.316-328, 2005.
  18. H. Khandelia, Y. Kaznessis, "Molecular dynamics simulations of the helical antimicrobial peptide ovipirin-1 in zwitterionic dodecylphosphocholine micelles: Insights into host-cell toxicity" *Journal of Physical Chemistry B*, Vol. 109(26) p. 12990 – 12996, 2005.
  19. V. Reddy, Y. Kaznessis, "Quantitative analysis of interfacial amino acid conservation in protein-protein hetero complexes" *Journal of Bioinformatics and Computational Biology*, Vol. 3(5), p.1137-50, 2005.
  20. H. Khandelia, Y. Kaznessis, "Molecular dynamics simulations of helical antimicrobial peptides in SDS micelles: What do point mutations achieve?" *Peptides*, Vol. 26(11), p. 2037-2049, 2005.
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21. H. Salis, Y. Kaznessis "An equation-free probabilistic steady state approximation: Dynamic application to the stochastic simulation of biochemical reaction networks", *Journal of Chemical Physics*, Vol. 123(21), p. 214106, 2005
  22. A. Langham, H. Khandelia, Y. Kaznessis, "How can protegrin-1 be both a potent antimicrobial and harmfully toxic?: Molecular dynamics simulations of a beta-sheet antimicrobial peptide in micelles" *Biopolymers: Peptide Science*, Vol. 84 (2), p.219-231, 2006.
  23. L. Tuttle, H. Salis, J. Tomshine, Y. Kaznessis, "Model-Driven Design Principles of Gene Networks: the Oscillator", *Biophysical Journal*, Vol. 89(6), p. 3873-83, 2005
  24. Y. Kaznessis, "Multi-Scale Models for Gene Network Engineering", *Chemical Engineering Science*, Vol. 61(3), p. 940-953, 2006.
  25. Y. Kaznessis, "A review of methods in computational prediction of blood-brain partitioning" *Current Medicinal Chemistry, Central Nervous System Agents*, Vol. 5, (3), p.185-191, 2005.
  26. H. Salis, V. Sotiropoulos, Y. Kaznessis "Multiscale Hy3S: Hybrid Stochastic Simulations for Supercomputers", *BMC Bioinformatics*, (highly accessed), Vol. 7:93, 2006.
  27. H. Khandelia, Y. Kaznessis, "Molecular Dynamics Investigation of the Influence of Anionic and Zwitterionic Interfaces on Antimicrobial Peptides' Structure: Implications on Peptide Toxicity and Activity" *Peptides*, Vol. 27(6), p.1192-1200, 2006.
  28. Y. Duan, B. Reddy, Y. Kaznessis "Residue conservation information for generating near-native structures in protein-protein docking" *Journal of Bioinformatics and Computational Biology*, 4:793-806, 2006.
  29. H. Khandelia, A. Langham, Y. Kaznessis, "Driving engineering of novel antimicrobial peptides from simulations of peptide-micelle interactions", *BBA, Biomembranes*, 1758(9):1224-34, 2006.
  30. W. Wang, C. Mulakala, S.C. Ward, G. Jung, H. Luong, D. Pham, A.J. Waring, Y. Kaznessis, W. Lu, K.A. Bradley, R.I. Lehrer. "Retrocyclins kill bacilli and germinating spores of *Bacillus anthracis* and inactivate anthrax lethal toxin." *Journal of Biological Chemistry*, 281(43):32755-64, 2006.
  31. J. Tomshine, Y. Kaznessis, "Optimization of a stochastically-simulated gene network model via simulated annealing," *Biophysical Journal*, *Biophys J.* 91(9):3196-205, 2006.
  32. A. Langham, Y. Kaznessis "Effects of mutations on the C-terminus of protegrin-1: a molecular dynamics simulation study", *Molecular Simulation*, 32(3-4):193-201, 2006.
  33. H. Salis, Y. Kaznessis, "Computer-aided design of modular protein devices: Boolean AND gene activation." *Phys Biol.* 3(4):295-310, 2006.
  34. V. Sotiropoulos, Y. Kaznessis, "Synthetic tetracycline-inducible regulatory networks: computer-aided design of dynamic phenotypes" *BMC Systems Biology*, 1:7, 2007
  35. C. Mulakala, J.D. Lambris, Y. Kaznessis, "A simple, yet highly accurate, QSAR model captures the complement inhibitory activity of compstatin", *Bioorg Med Chem.* 15(4):1638-44, 2007.
  36. H. Khandelia, Y. Kaznessis, "Structure of the Antimicrobial  $\beta$ -hairpin Peptide Protegrin-1 in a DLPC Lipid Bilayer Investigated by Molecular Dynamics Simulation", *BBA Biomembranes*, 1768(3):509-20, 2007.
  37. H. Khandelia, Y. Kaznessis, "Cation- $\pi$  Interactions Stabilize the Structure of the Antimicrobial Peptide Indolicidin near Membranes: Molecular Dynamics Simulations", *J. Phys. Chem. B*, 111(1):242-250, 2007
  38. D. Bolintineanu, A. Langham, T.H. Davis, Y. Kaznessis, "Molecular dynamics simulations of three protegrin-type anti-microbial peptides: interplay between charges at the termini,  $\beta$ -sheet structure and amphiphilic interactions", *Molecular Simulation*, 2007, 33, 809 – 819.
  39. A. Langham, A.J. Waring, Y. Kaznessis, "Comparison of interactions between  $\beta$ -hairpin decapeptides and SDS/DPC micelles from experimental and simulation data", *BMC Biochemistry*, 2007 Jul 16;8(1):11.
  40. S. Vicatos, Y. Kaznessis, "Separating true positive predicted residue contacts from false positive ones in mainly alpha proteins, using constrained Metropolis MC simulations." *Proteins*, 2008 Feb 1;70(2):539-52
  41. V. Sotiropoulos, Y.N. Kaznessis "An Adaptive Time Step Scheme for a System of SDE's with Multiple Multiplicative Noise. Chemical Langevin Equation, a proof of concept", *J. Chem. Phys.* 2008 Jan 7;128(1):014103.
  42. Reddy BV, Kaznessis YN. "Use of secondary structural information and C alpha-C alpha distance restraints to model protein structures with MODELLER." *J Biosci.* 2007 Aug;32(5):929-36.
  43. Kaznessis YN. "Models for synthetic biology." *BMC Syst Biol.* 2007 Nov 6;1(1):47
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44. Langham A., Sayyed-Ahmad A, Kaznessis YN, "On the nature of antimicrobial activity: a model for Protegrin-1 pores", JACS, in press

### Chapters in Books

Y. N. Kaznessis, R.G. Larson, "Molecular mechanics simulations and bioinformatics calculations in the study of lung surfactants". Invited chapter in the book "Recent Research Developments in Lung Surfactant and its Dysfunction" Edited by Kaushik Nag, Marcel-Dekker. New York, 2005.

### Invited and Conference Presentations since 2005

- Y. Kaznessis, "Synthetic Bio-logical AND gates", Synthetic Biology 3.0, Zurich, Switzerland, July 2007.
  - Y. Kaznessis, "Synthetic Bio-logical AND gates", Pathways, Networks and Systems Biology, Porto Heli, Greece, July 2007.
  - Y. Kaznessis, "Model-Driven Synthetic Bioengineering", PPEPPED 2007, Crete, Greece, June 2007.
  - A. Langham, "Computer-Driven Antimicrobial Peptide, Engineering", 2007 Biophysical Meeting, Baltimore, March 2007.
  - Howard Salis, Yiannis N. Kaznessis, "Bifurcation Analysis of Stochastic Gene Networks", American Institute of Chemical Engineers Annual Meeting, San Francisco, CA, November 2006.
  - Vassilios Sotiropoulos, Marie-Nathalie Contou-Carrere, Prodromos Daoutidis, Yiannis N. Kaznessis, "Reduction of Multi-Scale Systems of Chemical Langevin Equations", American Institute of Chemical Engineers Annual Meeting, San Francisco, CA, November 2006.
  - Himanshu Khandelia, Yiannis N. Kaznessis, "Molecular Dynamics Simulations to Guide the Design of Peptide Antibiotics", American Institute of Chemical Engineers Annual Meeting, San Francisco, CA, November 2006.
  - Howard Salis, Yiannis N. Kaznessis, "Computer Aided Design of Modular Protein Devices: Logical "and" Gene Activation, American Institute of Chemical Engineers Annual Meeting, San Francisco, CA, November 2006.
  - Abdallah Sayyed-Ahmad, Yiannis Kaznessis, "Relative Binding Free Energy Calculations of Antimicrobial Peptides in Sds/Dpc Micelles Using Molecular Dynamics/Continuum Methods", American Institute of Chemical Engineers Annual Meeting, San Francisco, CA, November 2006.
  - Allison Langham, Yiannis N. Kaznessis, "The Design of New Protegrin-like Antimicrobial Peptides: a Molecular Dynamics Study", American Institute of Chemical Engineers Annual Meeting, San Francisco, CA, November 2006.
  - Jonathan R. Tomshine, Yiannis N. Kaznessis, "Optimization of Stochastically-Simulated Gene Network Models", American Institute of Chemical Engineers Annual Meeting, San Francisco, CA, November 2006.
  - Spyridon Vicatos, Yiannis Kaznessis, " Separating True Positive Residue Contacts from False Positive Ones in Proteins, Using Constrained Metropolis Monte Carlo Simulations", American Institute of Chemical Engineers Annual Meeting, San Francisco, CA, November 2006.
  - Vassilios Sotiropoulos, Yiannis N. Kaznessis, "In Silico Design of Synthetic Tetracycline-Inducible Regulatory Gene Networks", American Institute of Chemical Engineers Annual Meeting, San Francisco, CA, November 2006.
  - Y. Kaznessis, "The New Mathematics of Biological Engineering, " presentation, International Conference in Bioengineering and Nanotechnology, Santa Barbara, CA, September, 2006.
  - H. Salis, Y. Kaznessis, "Multi-Scale Models for Gene Network Engineering", Raleigh, NC, August, 2006
  - Y. Kaznessis, "The New Mathematics of Biological Engineering", invited presentation, Iowa State University, April 2006.
  - A. Langham, Y. Kaznessis, "Simulations of Protegrin-1, a potent antimicrobial peptide", Biophysical Society Meeting, San Francisco, CA, 2006
  - H. Khandelia, Y. Kaznessis "Molecular Dynamics Simulations of Antimicrobial Peptides" Platform presentation, American Chemical Society, Atlanta, GA, 2006
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- A. Langham, Y. Kaznessis, "Simulations of Protegrin-1, a potent antimicrobial peptide", Biophysical Society Meeting, San Francisco, CA, 2006
- H. Salis, Y. Kaznessis, "Model-Driven Designs of Gene Regulatory Networks", Platform presentation, Biophysical Society Meeting, San Francisco, CA, 2006
- H. Khandelia, Y. Kaznessis "Molecular Dynamics Simulations of Antimicrobial Peptides" Platform presentation, Biophysical Society Meeting, San Francisco, CA, 2006
- Y. Kaznessis, "Multiscale Models for Gene Network Engineering", invited presentation, National Technical University, Athens, Greece, January 2006

### Membership

American Institute of Chemical Engineers, American Biophysical Society

### Professional Activities - Service

- Director, University of Minnesota Bioinformatics Summer Institute
- Editorial Board, BMC Systems Biology
- Director, AIChE FPBE Division
- Fellow, Minnesota Supercomputing Institute
- Member, Steering Committee, University of Minnesota Computational Genetic Laboratory
- **Past service:** Vice Chair, Computational Genomics, 2006 AIChE Annual Meeting; Member, Graduate Admissions Committee, CEMS; Member, Organizing Committee, 2007 Bioengineering Conference; Member, Organizing Committee, 2005 Foundations of Systems Biology and Engineering Conference; Member, Advisory Committee, University of Minnesota Digital Technology Center; Member, NIH Review Panel, NIH Pathway to Independence Award; Member, NSF Partnership for Advanced Computational Infrastructure Committee; Vice Chair, Biomedical Applications of Systems Biology Session, 2005 AIChE Annual Meeting; Member, Faculty Recruiting Committee, Department of Computer Science and Engineering; Member, Chemical Engineering Curriculum Committee (2003), CEMS; Vice Chair, Bioinformatics Topical Conference, 2001 AIChE Annual Meeting; Chair, Group T3, Bioinformatics, 2002 AIChE Annual Meeting; Member, NSF SBIR 2004 panel; Member, NSF Emerging Models and Technologies (EMT) 2004 and 2005 panels
- Reviewer of manuscripts in: Biophysical Journal, Biological Macromolecules, Biochimica & Biophysica Acta, Bioorganic and Medicinal Chemistry, BMC Bioinformatics, Biotechnology and Bioengineering, Computers and Chemical Engineering, Journal of Biotechnology, Journal of Physical Chemistry, Journal of Chemical Physics, Langmuir, Molecular Simulation, Physical Biology, Proteins.

### Research Group

**Graduate students:** Katherine Volzing, Apostolos Vagias, Allison Langham, Jonathan Tomshine, Vassilis Sotiropoulos, Dan Bolintineanu, John Barrett, Nagendra Singh, Anushree Chatterjee

**Postdoctoral Fellows:** Abdallah Sayyed-Ahmad, Ting-Lan Chiu, Chandrika Mulakala, Anthony Hill, Kavita Iyer, Poonam Shrivastave

### Past Group Members

Spyros Vicatos (Ph.D. 2007) now postdoctoral fellow at the University of Southern California.  
 Himanshu Khandelia (Ph.D. 2006) now postdoctoral fellow at the University of Southern Denmark  
 Howard Salis (Ph.D. 2007) now postdoctoral fellow at the University of California, San Francisco  
 Nathan Ostberg (M.Sc), Lisa Tuttle (BSI and M.Sc.), Yuhua Duan (postdoctoral fellow, now at DOE National Energy Technology Laboratory), Boojala Reddy (research associate, now assistant professor at CUNY), Hairong Wei (postdoctoral fellow, now research associate at the University of Alabama). Another four chemical engineering undergraduate students have worked in our group, along with seventeen Bioinformatics Summer Institute interns.