In Memoriam: Christodoulos Achilleus Floudas

Ruth Misener

Department of Computing,
Imperial College London
South Kensington SW7 2AZ, UK

r.misener@imperial.ac.uk

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The Centre for Process Systems Engineering (CPSE) lost a terrific research collaborator and a dear friend this summer. Professor Christodoulos Achilleus Floudas passed away of an apparent heart attack on 14 August 2016 while vacationing in Greece with his family. Chris is survived by his wife, Fotini, and their daughter, Ismini. Born 31 August 1959 in Ioannina, Greece, Chris earned a Diploma of Chemical Engineering at the Aristotle University of Thessaloniki in 1982, and a PhD in chemical engineering from Carnegie Mellon University in 1986. Chris subsequently moved to Princeton University where he served 29 years and, in 2007, was appointed *Stephen C. Macaleer '63 Professor in Engineering and Applied Science*. In 2015, Chris moved to Texas A&M University where he was appointed *Director* of the Texas A&M Energy Institute and *Erle Nye '59 Chair Professor for Engineering Excellence* at the Artie McFerrin Department of Chemical Engineering.

To name only a few of his accolades, Chris was a Member of the National Academy of Engineering (2011), a SIAM Fellow (2013), a Thompson Reuters Highly Cited Researcher in two consecutive years (2014, 15), and a Corresponding Member of the Academy of Athens (2015). Chris was also an outstanding mentor and teacher. In 2007, Chris became the first recipient of Princeton University's (now annual) Graduate Mentoring Award; recognition for his teaching includes the Princeton University Engineering Council Teaching Award (1995) and the Aspen Tech Excellence in Teaching Award (1999). He has supervised 34 PhD students to completion and 20 postdoctoral research associates; many of these are now internationally-leading researchers or professors. Nine further PhD students are working on their degrees.[1]

Professor Floudas had broad and deep connections to CPSE. Three of Chris's former PhD students, Claire Adjiman, Peter DiMaggio, and Ruth Misener, are now CPSE academic faculty. Five researchers with PhDs from the centre launched their postdoctoral careers in Chris's Princeton-based laboratory: Vassilios Vassiliadis (PhD 1993), Marianthi Ierapetritou (PhD 1995), Ioannis Akrotirianakis (PhD 2000), Frances Pereira (PhD 2010), and Wolfram Wiesemann (PhD 2010). Prof. Stratos Pistikopoulos, who was a CPSE academic for 23 years and led the centre for 8 years, left CPSE in 2015 to become *Associate Director* of the Texas A&M Energy Institute where Chris was *Director*. Chris's frequent visits to the centre were exceptionally productive, e.g. his autumn 1992 sabbatical led to the book *Nonlinear and Mixed-Integer Optimization: Fundamentals and Applications* [1]. Chris delivered the 2008 *Professor Roger Sargent Lecture*, was PhD examiner for many students including Ioannis Papamichail (2002) and Polyxeni-M. Kleniati (2009), and gave the *Vote of Thanks* for the inaugural of Prof. Claire Adjiman.

This reflection discusses some of the contributions Chris made to mathematical optimization, with a particular emphasis on deterministic global optimization. Our central thesis is that **Professor Floudas fundamentally opened the field of deterministic global optimization, making the discipline industrially-relevant and blazing a path where subsequent research could follow.** His unforgettable contribution is to drive mathematical optimization towards everyday relevance: he pushed the tractability boundary of optimization theory, algorithms, and implementations

[1] Professor Floudas' academic tree: http://titan.engr.tamu.edu/tree/caf/

using a multitude of applications.

Chris's PhD thesis, supervised by Professor Ignacio Grossmann at CMU, investigated the automatic synthesis of heat exchanger networks [2]. Designing heat exchanger networks is a mixed-integer nonlinear program (MINLP) with long-reaching implications for energy efficiency; a quarter of the EU 2012 energy consumption came from industry and industry uses 73% of this energy on heating and cooling [3]. Chris's contribution was to derive many possible superstructures from a mixed-integer linear programming (MIP) approximation of the MINLP, fix the binary decision variables, and locally solve the resulting nonlinear program (NLP). Chris also used flexibility analysis to design networks that can handle uncertain flowrates and temperatures. Flexibility analysis is a max-min-max optimization problem quantifying how far parameters can deviate from their nominal values while maintaining operational feasibility [4]; the closest analogue in modern-day mathematical programming research is robust optimization [5].

Chris developed a passion for deterministic global optimization soon after he started as an assistant professor in Princeton University's Department of Chemical Engineering in 1986. He and his early students developed the Global Optimization Algorithm (GOP), an extension of Generalized Benders Decomposition applicable to biconvex optimization problems [6–8]. Rigorous global optimization was not new, but Chris was the first to develop global optimization methodology and then apply these algorithms to important classes of nonconvex nonlinear chemical engineering problems including the pooling problem [9] and phase equilibrium [10].

Chris's interest in computational chemistry led him to develop αBB, a convexification methodology based on the difference of convex functions. Energy minimization plays a central role in understanding and predicting the behavior of natural systems. Using an application to Lennard-Jones microclusters [11], Chris and Costas Maranas became the first to apply rigorous global optimization to molecular thermodynamics; energy minimisation using local rather than global optimization may yield significant qualitative and quantitative errors in engineering decision making [12]. To find the global minimum energy configuration of Lennard-Jones microclusters, Maranas and Floudas [11] transformed the optimization problem, with its nonconvex pair potential term $\left(1/r^{12} - 2/r^6\right)$, into a difference-of-convex (DC) program using a sufficiently large parameter $\alpha > 0$ multiplied by a quadratic function. In autumn 1992, Chris took a sabbatical at Imperial College London where, with Wenbin Liu, he generalized the Maranas and Floudas [11] result to any nonconvex function with a Lipschitz continuous gradient [13]. These results led to the now-famous αBB (α-branch-and-bound) convexification methodology where a convex lower bounding function $g^{\text{cnv}}(\mathbf{x})$ can be defined for generic nonconvex function $g(\mathbf{x})$ with the addition of a separable convex quadratic function [14]:

$$g^{\text{cnv}}(\mathbf{x}) = g(\mathbf{x}) - \sum_i \alpha_i (x_i^U - x_i)(x_i - x_i^L)$$
$$\text{where } \alpha_i \geq \max\left\{0, -\frac{1}{2} \min_{\mathbf{x}^L \leq \mathbf{x} \leq \mathbf{x}^U} \lambda(\mathbf{x})\right\}.$$

Chris and his co-workers developed protocols to automatically calculate the α parameters and implemented αBB-based global optimization as a generic MINLP solver [14–16]. Subsequent advances in αBB theory identified alternative univariate exponential perturbations [17], piecewise underestimators [18, 19], and nondiagonal αBB [20, 21]. The dependence on the eigenvalues λ of the Hessian matrix of the second derivatives of $g(\mathbf{x})$ has inspired further investigatation into Hessian matrix spectral bounds [22].

The MINLP solver implementing the αBB methodology, written with Claire Adjiman and Yannis Androulakis [23], became Chris's major vehicle to approach a wide variety of applications: parameter estimation [24, 25], optimal control [26], reactor network synthesis [27], semi-infinite programming [28], bilevel programming [29], molecular structure prediction [30], peptide and protein folding [31–36], design under uncertainty [37], solving constrained systems of equations [38], phase equilibrium calculations [10, 39–41], and solving subproblems within an augmented Lagrangian framework [42]. In many of these domains, Chris was the first researcher to even attempt applying global optimization.

But Chris was never interested in toy problems or proofs-of-concept; if he was going to apply mathematical optimization to a new problem class, he would always push optimization to its limit via highly-relevant, industrially-motivated test cases. For example, the problem of *de novo* peptide design begins with a flexible, 3D protein structure and finds amino acid sequences folding into the given template; the possible impact on both fundamentally understanding protein structure and developing novel therapeutics is enormous [43, 44]. The first stage of Chris's *de novo* peptide design framework is to develop many possible amino acid sequences; Chris and his co-workers identified a deep connection with the Quadratic Assignment Problem (QAP) and adapted QAP solution techniques to the specific problem [45, 46]. In the second stage, Chris and his co-workers apply their ASTRO-FOLD technology (which uses αBB) to generate a 3D peptide structure [31–36]. This framework for *de novo* peptide design has been applied to several therapeutic applications including cancer [47] and HIV [48, 49].

Energy systems engineering is another domain that inspired Chris to make fundamental mathematical optimization contributions. As with molecular biology, Chris's complete refusal to address anything but the most pressing, real-world problems led him to the tractability boundary of mathematical optimization. Together with Rich Baliban and Josephine Elia, Chris designed an optimization framework for the simultaneous process synthesis, heat and power integration of a thermochemical hybrid biomass, coal, and natural gas facility [50]. Then Chris wanted to globally optimize a model with 15,439 continuous variables, 30 binary variables, 15,406 equality constraints, 230 inequality constraints, and 335 nonconvex terms [51]. But Chris absolutely insisted that his piecewise linear underestimation technique for bilinear terms [52–54] was not relevant unless it was effectively applied to real-world instances; since that time Chris and his co-workers have applied a similar methodology to pressing applications such as designing biomass-based production of chemicals and fuels [55–57] or transforming municipal solid waste to liquid fuel [58].

The difficulty of the aforementioned energy systems applications is primarily rooted in the nonconvex bilinear terms, e.g. $f \cdot c$, that arise with intermediate storage in process networks [59]. The special structure of the so-called *pooling problem* is incredibly interesting: flow variables f are multiplied by concentration variables c and an undirected graph representation of the bilinear terms (where the decision variables are the nodes and the connecting edges are weighted by the coefficients) is bipartite [60]. Chris had made major contributions to this problem since 1990 [9], but one of his more recent intuitions was that piecewise linear underestimators seemed to be effective in solving the pooling problem [52–54].

Chris developed, with Cliff Meyer, several important results on the facets of the trilinear monomials [61, 62]. Chris and Cliff further generalized these results to automatically generate the facets of *edge-concave functions*, e.g. those admitting a vertex polyhedral envelope [63]. One of the projects with Ruth Misener extended the Meyer and Floudas [63] methodology to develop multiterm underestimators for bilinear functions [60].

Chris and Ruth released first GloMIQO [64] and then ANTIGONE [65] as global optimization solvers in the modeling language GAMS. The solver incorporates several contributions Chris and his co-workers made including those to: αBB [15], generalised geometric programming [66, 67], edge-concave underestimators [63, 68], and automatic transformations for process networks problems [60, 64]. One application of ANTIGONE was in Chris developing, with Fani Boukouvala and Faruque Hasan, a general methodology for grey-box models [69]. Chris had previously developed approaches in black-box optimization [70], i.e. optimization for functions without explicit analytical representation, but his new work is especially exciting because it develops optimization methodology for applications where some of the governing equations are known but others have to be determined using a data-driven methodology [71]. Chris and his co-workers used this methodology to develop a global optimization framework for entire petrochemical planning operations [72].

This reflection on the contributions of Chris to mathematical optimization has been (necessarily) brief, but we should mention some of the contributions that Chris made to optimization under uncertainty. Chris first encountered uncertainty in synthesizing heat exchanger networks with uncertain flowrates and temperatures [4] and uncertainty was thereafter a thread that ran throughout his research [73]. Chris's early work in optimization under uncertainty was mostly in *flexibility* [37], but he later became keenly interested in robust optimization and introduced the methodology to the chemical engineering community [74–77]. In particular, Chris and his co-workers extended robust optimization, which was originally developed as a convex optimization methodology, to important nonconvex problems including operational planning [78], crude oil scheduling [79], and the vehicle routing problem [80].

The contributions Chris made to mathematical optimization are legion, but his contributions also extended to supporting the work of many other global optimizers. Together with Panos Pardalos, Chris and his students published the *Handbook of Test Problems in Local and Global Optimization* which has become a standard test set for any global optimization solver [81]. Floudas and Pardalos edited many other special issues and books together [82–86]; the most significant is the *Encyclopedia of Optimization* [87]. These books brought significant attention to deterministic global optimization and supported the careers of many researchers. Finally, we should conclude by mentioning the close friendship between Chris and Stratos Pistikopoulos; the two met as undergraduates and forged a tight connection while both were PhD students at CMU. They were collaborators [8, 73, 88, 89], but another lasting result of Chris and Stratos' friendship was their roles as founding *Director* and *Associate Director*, respectively, of the Texas A&M Energy Institute. There the work of Chris continues: the PhD students of Chris are all keen to continue with Stratos the work they started with Chris.

May his memory be eternal.

References

[1] Floudas. *Nonlinear and Mixed-Integer Optimization: Fundamentals and Applications*. Oxford University Press, New York, NY, 1995.

[2] Floudas, Ciric, and Grossmann. Automatic synthesis of optimum heat exchanger network configurations. *AIChE J*, 32(2):276–290, 1986.

[3] European Commission. An EU strategy on heating and cooling, 2016. Brussels, COM(2016) 51 final.

[4] Floudas and Grossmann. Synthesis of flexible heat-exchanger networks with uncertain flowrates and temperatures. *Comput Chem Eng*, 11(4):319–336, 1987.

[5] Zhang, Grossmann, and Lima. On the relation between flexibility analysis and robust optimization for linear systems. *AIChE J*, 62(9):3109–3123, 2016.

[6] Floudas and Visweswaran. A global optimization algorithm (GOP) for certain classes of nonconvex NLPs: I. Theory. *Comput Chem Eng*, 14(12):1397–1417, 1990.

[7] Floudas and Visweswaran. Primal-relaxed dual global optimization approach. *J Optim Theory Appl*, 78(2):187–225, 1993.

[8] Visweswaran, Floudas, Ierapetritou, and Pistikopoulos. A decomposition-based global optimization approach for solving bilevel linear and quadratic programs. In Floudas and Pardalos, editors, *State of the Art in Global Optimization: Computational Methods and Applications*, volume 7 of *Nonconvex Optimization and its Applications*, pages 139–162, 1996.

[9] Visweswaran and Floudas. A global optimization algorithm (GOP) for certain classes of nonconvex NLPs: II. application of theory and test problems. *Comput Chem Eng*, 14(12):1419–1434, 1990.

[10] McDonald and Floudas. Decomposition based and branch and bound global optimization approaches for the phase equilibrium problem. *J Glob Optim*, 5:205–251, 1994.

[11] Maranas and Floudas. A global optimization approach for Lennard-Jones microclusters. *J Chem Phys*, 97(10):7667–7678, 1992.

[12] Bollas, Barton, and Mitsos. Bilevel optimization formulation for parameter estimation in vapor-liquid(-liquid) phase equilibrium problems. *Chem Eng Sci*, 64(8):1768–1783, 2009.

[13] Liu and Floudas. A remark on the GOP algorithm for global optimization. *J Glob Optim*, 3:519–521, 1993.

[14] Androulakis, Maranas, and Floudas. αBB: A global optimization method for general constrained nonconvex problems. *J Glob Optim*, 7:337–363, 1995.

[15] Adjiman, Dallwig, Floudas, and Neumaier. A global optimization method, αBB, for general twice differentiable NLPs-I. Theoretical advances. *Comput Chem Eng*, 22:1137–1158, 1998.

[16] Adjiman, Androulakis, and Floudas. A global optimization method, αBB, for general twice differentiable NLPs-II. Implementation and computational results. *Comput Chem Eng*, 22:1159–1179, 1998.

[17] Akrotirianakis and Floudas. Computational experience with a new class of convex underestimators: Box-constrained NLP problems. *J Glob Optim*, 29(3):249–264, 2004.

[18] Meyer and Floudas. Convex underestimation of twice continuously differentiable functions by piecewise quadratic perturbation: Spline αBB underestimators. *J Glob Optim*, 32(2):221–258, 2005.

[19] Gounaris and Floudas. Tight convex underestimators for $\mathcal{C}^2$-continuous problems: II. Multivariate functions. *J Glob Optim*, 42(1):69–89, 2008.

[20] Akrotirianakis, Meyer, and Floudas. The role of the off-diagonal elements of the Hessian matrix in the construction of tight convex underestimators for nonconvex functions. In *Discovery Through Product and Process Design*, pages 501–504. Foundations of Computer-Aided Process Design, 2004.

[21] Skjäl, Westerlund, Misener, and Floudas. A generalization of the classical αBB convex underestimation via diagonal and nondiagonal quadratic terms. *J Optim Theory Appl*, 154(2):462–490, 2012.

[22] Mönnigmann. Efficient calculation of bounds on spectra of Hessian matrices. *SIAM J Sci Comput*, 30(5):2340–2357, 2008.

[23] Adjiman, Androulakis, and Floudas. Global optimization of mixed-integer nonlinear problems. *AIChE J*, 46(9):1769–1797, 2000.

[24] Esposito and Floudas. Global optimization in parameter estimation of nonlinear algebraic models via the error-in-variables approach. *Ind Eng Chem Res*, 37:1841–1858, 1998.

[25] Esposito and Floudas. Global optimization for the parameter estimation of differential-algebraic systems. *Ind Eng Chem Res*, 39(5):1291–1310, 2000.

[26] Esposito and Floudas. Deterministic global optimization in nonlinear optimal control problems. *J Glob Optim*, 17:97–126, 2000.

[27] Esposito and Floudas. Deterministic global optimization in isothermal reactor network synthesis. *J Glob Optim*, 22(1-4):59–95, 2002.

[28] Floudas and Stein. The adaptive convexification algorithm: A feasible point method for semi-infinite programming. *SIAM J Optim*, 18(4):1187–1208, 2007.

[29] Gümüs and Floudas. Global optimization of nonlinear bilevel programming problems. *J Glob Optim*, 20(1):1–31, 2001.

[30] Maranas and Floudas. A deterministic global optimization approach for molecular-structure determination. *J Chem Phys*, 100(2):1247–1261, 1994.

[31] Klepeis and Floudas. Free energy calculations for peptides via deterministic global optimization. *J Chem Physics*, 110:7491–7512, 1999.

[32] Klepeis and Floudas. Deterministic global optimization and torsion angle dynamics for molecular struc-

ture prediction. *Comput Chem Eng*, 24(2-7):1761–1766, 2000.

[33] Klepeis and Floudas. Ab initio tertiary structure prediction of proteins. *J Glob Optim*, 25:113–140, 2003.

[34] Klepeis and Floudas. ASTRO-FOLD: a combinatorial and global optimization framework for ab initio prediction of three-dimensional structures of proteins from the amino acid sequence. *Biophysical J*, 85:2119–2146, 2003.

[35] Klepeis, Floudas, Morikis, and Lambris. Predicting peptide structures using NMR data and deterministic global optimization. *J Comput Chem*, 20(13):1354–1370, 1999.

[36] Klepeis, Pieja, and Floudas. A new class of hybrid global optimization algorithms for peptide structure prediction: Integrated hybrids. *Comput Phys Commun*, 151:121–140, 2003.

[37] Floudas, Gümüs, and Ierapetritou. Global optimization in design under uncertainty: Feasibility test and flexibility index problems. *Ind Eng Chem Res*, 40(20):4267–4282, 2001.

[38] Maranas and Floudas. Finding all solutions of nonlinearly constrained systems of equations. *J Glob Optim*, 7(2):143–182, 1995.

[39] McDonald and Floudas. Global optimization for the phase and chemical equilibrium problem: Application to the NRTL equation. *Comput Chem Eng*, 19(11):1111–1141, 1995.

[40] McDonald and Floudas. Global optimization for the phase stability problem. *AIChE J*, 41(7):1798–1814, 1995.

[41] McDonald and Floudas. Global optimization and analysis for the Gibbs free energy function for the UNIFAC, Wilson, and ASOG equations. *Ind Eng Chem Res*, 34:1674–1687, 1995.

[42] Birgin, Floudas, and Martínez. Global minimization using an augmented Lagrangian method with variable lower-level constraints. *Math Program*, 125:139–162, 2010.

[43] Floudas, Fung, McAllister, Mönnigmann, and Rajgaria. Advances in protein structure prediction and de novo protein design: A review. *Chem Eng Sci*, 61(3):966–988, 2006.

[44] Khoury, Smadbeck, Kieslich, and Floudas. Protein folding and de novo protein design for biotechnological applications. *Trends in Biotechnology*, 32(2):99–109, 2014.

[45] Klepeis, Floudas, Morikis, Tsokos, and Lambris. Design of peptide analogues with improved activity using a novel de novo protein design approach. *Ind Eng Chem Res*, 43(14):3817–3826, 2004.

[46] Fung, Rao, Floudas, Prokopyev, Pardalos, and Rendl. Computational comparison studies of quadratic assignment like formulations for the in silico sequence selection problem in de novo protein design. *J Comb Optim*, 10(1):41–60, 2005.

[47] Smadbeck, Peterson, Zee, Garapaty, Mago, Lee, Giannis, Trojer, Garcia, and Floudas. De novo peptide design and experimental validation of histone methyltransferase inhibitors. *PLoS One*, 9(2):e90095, 2014.

[48] Bellows and Floudas. Computational methods for de novo protein design and its applications to the human immunodeficiency virus 1, purine nucleoside phosphorylase, ubiquitin specific protease 7, and histone demethylases. *Curr Drug Targets*, 11:264–278, 2010.

[49] Kieslich, Tamamis, Guzman, Onel, and Floudas. Highly accurate structure-based prediction of HIV-1 coreceptor usage suggests intermolecular interactions driving tropism. *PLoS ONE*, 11(2):1–15, 2016.

[50] Baliban, Elia, and Floudas. Optimization framework for the simultaneous process synthesis, heat and power integration of a thermochemical hybrid biomass, coal, and natural gas facility. *Comput Chem Eng*, 35(9):1647–1690, 2011.

[51] Baliban, Elia, Misener, and Floudas. Global optimization of a MINLP process synthesis model for thermochemical based conversion of hybrid coal, biomass, and natural gas to liquid fuels. *Comput Chem Eng*, 42:64–86, 2012.

[52] Meyer and Floudas. Global optimization of a combinatorially complex generalized pooling problem. *AIChE J*, 52(3):1027–1037, 2006.

[53] Gounaris, Misener, and Floudas. Computational comparison of piecewise-linear relaxations for pooling problems. *Ind Eng Chem Res*, 48(12):5742–5766, 2009.

[54] Misener, Thompson, and Floudas. APOGEE: Global optimization of standard, generalized, and extended pooling problems via linear and logarithmic partitioning schemes. *Comput Chem Eng*, 35(5):876–892, 2011.

[55] Niziolek, Onel, Elia, Baliban, Xiao, and Floudas. Coal and biomass to liquid transportation fuels: Process synthesis and global optimization strategies. *Ind Eng Chem Res*, 53(44):17002–17025, 2014.

[56] Matthews, Niziolek, Onel, Pinnaduwage, and Floudas. Biomass to liquid transportation fuels via biological and thermochemical conversion: Process synthesis and global optimization strategies. *Ind Eng Chem Res*, 55(12):3203–3225, 2016.

[57] Niziolek, Onel, Guzman, and Floudas. Biomass-based production of benzene, toluene, and xylenes via methanol: Process synthesis and deterministic global optimization. *Energy Fuels*, 30(6):4970–4998, 2016.

[58] Niziolek, Onel, and Floudas. Municipal solid waste to liquid transportation fuels, olefins, and aromatics: Process synthesis and deterministic global optimization. *Comput Chem Eng*, 2016. DOI: 10.1016/j.compchemeng.2016.07.024.

[59] Misener and Floudas. Advances for the pooling problem: Modeling, global optimization, and computational studies. *Appl Comput Math*, 8(1):3–22, 2009.

[60] Misener, Smadbeck, and Floudas. Dynamically-generated cutting planes for mixed-integer quadratically-constrained quadratic programs and their incorporation into GloMIQO 2.0. *Optim Met Softw*, 30(1):215–249, 2014.

[61] Meyer and Floudas. Trilinear monomials with positive or negative domains: Facets of the convex and concave envelopes. In Floudas and Pardalos, editors, *Frontiers in Global Optimization*, pages 327–352. Kluwer, 2003.

[62] Meyer and Floudas. Trilinear monomials with mixed sign domains: Facets of the convex and concave envelopes. *J Glob Optim*, 29(2):125–155, 2004.

[63] Meyer and Floudas. Convex envelopes for edge-concave functions. *Math Program*, 103(2):207–224, 2005.

[64] Misener and Floudas. GloMIQO: Global Mixed-Integer Quadratic Optimizer. *J Glob Optim*, 57(1):3–50, 2013.

[65] Misener and Floudas. ANTIGONE: Algorithms for coNTinuous Integer Global Optimization of Nonlinear Equations. *J Glob Optim*, 59(2-3):503–526, 2014.

[66] Maranas and Floudas. Global optimization in generalized geometric programming. *Comput Chem Eng*, 21(4):351–369, 1997.

[67] Misener and Floudas. A framework for globally optimizing mixed-integer signomial programs. *J Optim Theory Appl*, 161:905–932, 2014.

[68] Misener and Floudas. Global optimization of mixed-integer quadratically-constrained quadratic programs (MIQCQP) through piecewise-linear and edge-concave relaxations. *Math Program*, 136:155–182, 2012.

[69] Boukouvala, Hasan, and Floudas. Global optimization of general constrained grey-box models: new method and its application to constrained PDEs for pressure swing adsorption. *J Glob Optim*, 2015. DOI: 10.1007/s10898-015-0376-2.

[70] Meyer, Floudas, and Neumaier. Global optimization with nonfactorable constraints. *Ind Eng Chem Res*, 41(25):6413–6424, 2002.

[71] Boukouvala and Floudas. Argonaut: Algorithms for global optimization of constrained grey-box computational problems. *Optim Lett*, 2016. DOI: 10.1007/s11590-016-1028-2.

[72] Li, Xiao, Boukouvala, Floudas, Zhao, Du, Su, and Liu. Data-driven mathematical modeling and global optimization framework for entire petrochemical planning operations. *AIChE J*, 62(9):3020–3040, 2016.

[73] Ierapetritou, Pistikopoulos, and Floudas. Operational planning under uncertainty. *Comput Chem Eng*, 20(12):1499–1516, 1996.

[74] Lin, Janak, and Floudas. A new robust optimization approach for scheduling under uncertainty: I. Bounded uncertainty. *Comput Chem Eng*, 28(6-7):1069–1085, 2004.

[75] Janak, Lin, and Floudas. A new robust optimization approach for scheduling under uncertainty: II. Uncertainty with known probability distribution. *Comput Chem Eng*, 31(3):171–195, 2007.

[76] Li and Floudas. Optimal scenario reduction framework based on distance of uncertainty distribution and output performance: I. Single reduction via mixed integer linear optimization. *Comput Chem Eng*, 70:50–66, 2014.

[77] Li and Floudas. Optimal scenario reduction framework based on distance of uncertainty distribution and output performance: II. Sequential reduction. *Comput Chem Eng*, 84:599–610, 2016.

[78] Verderame and Floudas. Operational planning of large-scale industrial batch plants under demand due date and amount uncertainty. I. Robust optimization framework. *Ind Eng Chem Res*, 48(15):7214–7231, 2009.

[79] Li, Misener, and Floudas. Scheduling of crude oil operations under demand uncertainty: A robust optimization framework coupled with global optimization. *AIChE J*, 58(8):2373–2396, 2012.

[80] Gounaris, Wiesemann, and Floudas. The robust capacitated vehicle routing problem under demand uncertainty. *Oper Res*, 61(3):677–693, 2013.

[81] Floudas, Pardalos, Adjiman, Esposito, Gümüs, Harding, Klepeis, Meyer, and Schweiger. *Handbook of Test Problems in Local and Global Optimization*. Kluwer, 1999.

[82] Floudas and Pardalos. State-of-the-art in global optimization - computational methods and applications - preface. *J Glob Optim*, 7(2):113, 1995.

[83] Floudas and Pardalos, editors. *State of the Art In Global Optimization: Computational Methods and Applications*. Kluwer, 1996.

[84] Floudas and Pardalos, editors. *Optimization in Computational Chemistry and Molecular Biology: Local and Global Approaches*. Nonconvex Optimization and Its Applications. Kluwer, 2000.

[85] Floudas and Pardalos, editors. *Frontiers in Global Optimization*. Nonconvex Optimization and Its Applications, Kluwer, 2004.

[86] Floudas and Pardalos, editors. *J Glob Optim*. 2009. *43*(2).

[87] Floudas and Pardalos. *Encyclopedia of optimization*. Springer Science & Business Media, 2001.

[88] Papalexandri, Pistikopoulos, and Floudas. Mass-exchange networks for waste minimization-a simultaneous approach. *Chem eng res design*, 72(3):279–294, 1994.

[89] Floudas and Pistikopoulos. Professor Ignacio E. Grossmann-Tribute. *Comput Chem Eng*, 72:1–2, 2015.