Andreas G. Boudouvis
Professor, former Rector
National Technical University of Athens
School of Chemical Engineering

CURRICULUM VITAE
June 2026

Born 28 January 1959, in the city of Pyrgos, Peloponnese, Greece. Married, father of a son and a daughter.

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EDUCATION

1987	PhD	Chemical Engineering	University of Minnesota, Minneapolis, USA

PhD Thesis title: *Mechanisms of surface instabilities and pattern formation in ferromagnetic liquids*. Thesis Advisor: Prof. L. E. Scriven

1982	Diploma	Chemical Engineering	National Technical University of Athens, Greece

PROFESSIONAL EXPERIENCE

9/2018	-	1/2019	*Visiting Professor,* Department of Chemical and Biomolecular Engineering, Johns Hopkins University, Baltimore, Maryland, USA
9-10/2016			*Visiting Professor*, Institut National Polytechnique de Toulouse, France
6-7/ 2014			*Invited Senior Researcher*, Ecole Nationale Supérieure des Ingénieurs en Arts Chimiques et Technologiques & Fondation de Cooperation Scientifique Sciences et Technologies pour l'Aéronautique et l'Espace, Toulouse, France
6-7/2012			*Visiting Professor*, Faculté des Sciences et Technologies, Université de Lorraine, Nancy, France
6/2005	-	present	*Professor*, School of Chemical Engineering, NTUA
6/2000	-	6/2005	*Associate Professor*, School of Chemical Engineering, NTUA
6/1998	-	6/2000	*Assistant Professor with tenure*, School of Chemical Engineering, NTUA
10/1994	-	6/1998	*Assistant Professor*, School of Chemical Engineering, NTUA
1/1991	-	10/1994	*Lecturer*, School of Chemical Engineering, NTUA
7/1991	-	9/1991	*Senior Visiting Research Fellow*, Army High Performance Computing Research Center, University of Minnesota, USA
11/1989	-	7/1990	*Postdoctoral Fellow*, Minnesota Supercomputer Institute, University of Minnesota, USA
3/1988	-	10/1989	*Engineering Scientist*, on duty in the Greek Army
8/1981	-	12/1987	*Graduate Research Assistant*, Department of Chemical Engineering and Materials Science, University of Minnesota, USA

ADMINISTRATIVE POSITIONS

NTUA:

10/2019	-	11/2023	*Rector* of the National Technical University of Athens
3/2013	-	8/2016	*Dean* of the School of Chemical Engineering, NTUA

9/2011	-	8/2018	*Director*, Inter-Departmental Graduate Studies Program "Computational Mechanics", NTUA
9/2009	-	10/2019	*Director*, Computer Center and PC Lab, School of Chemical Engineering, NTUA
9/2005	-	9/2007	*Head*, Department of Process Analysis & Plant Design, School of Chemical Engineering, NTUA

Abroad:
2021-2023**,** Co-Chairman, Presidents Board, European University "EULiST - European Universities Linking Society and Technology"; Since 2024, member of the EULiST Advisory Council.

2020- Board member, Hellenic Institute of Advanced Studies-HIAS

RESEARCH

Transport Phenomena, Interfacial Phenomena, Magneto-Electro-Fluid Mechanics, Nonlinear Phenomena, Large-Scale Scientific Computing, Multiscale Analysis, Reduced-Order Modeling/Machine Learning.

TEACHING

Undergraduate courses: Transport Phenomena, Computational Transport Phenomena, Advanced Fluid Mechanics, Computer Programming, Chemical Engineering Laboratory
Graduate courses: Computational Analysis with the Finite Element Method, Transport Phenomena, Advanced Transport Phenomena

STUDENT SUPERVISION
Graduate student supervision:
Advisor or co-advisor in *23 PhD theses* - 23 completed, 1 under way
Advisor in *50 Masters' theses*
Undergraduate student supervision: Advisor in *130 Diploma theses*

- Among the supervised PhD students, four are *faculty members in Greek universities*: A. G. Papathanasiou (PhD 2000) Professor in NTUA, A. Yiotis (PhD 2003) Assistant Professor in the Technical University of Crete, G. Kokkoris (PhD 2005) Associate Professor in NTUA and M. E. Kavousanakis (PhD 2007) Assistant Professor in NTUA.

The following supervised PhD or Diploma thesis students are recipients of a *European Research Council (ERC) Starting Grant: A. G. Papathanasiou* (PhD 2000) received an ERC grant in 2010; *C. Tsogka* – Diploma 1995, formerly Professor at Univ. of Crete, now at Univ. California – received an ERC grant in 2010; *T. Stylianopoulos* – Diploma 2003, now Associate Professor at Univ. of Cyprus – received an ERC grant in 2014 and in 2024.

HONORS AND AWARDS

2024	Recipient of the 2024 Award for Excellence in Academic Teaching. It is awarded by the Foundation for Research and Technology-Hellas in memory of V. Xanthopoulos and S. Pnevmatikos. On 18 December 2024, in the Hall of the Old Parliament in Athens, H. E. the President of the Hellenic Republic, Katerina Sakellaropoulou, presented the Award to A. G. Boudouvis - The ceremony.
2024	Dr E. Koronaki and the PhD candidates P. Papavasileiou and G. Suntaxi, researchers in our group, received the *Outstanding Scientific Achievement Award* from the *FNR*-

	National Research Fund of Luxembourg, as members of an interdisciplinary team from the University of Luxembourg and the advanced materials company Ceratizit. The achievement is about using hybrid equation-based and data-driven models that led to significant improvements in industrial coating processes with Chemical Vapor Deposition. More in the NTUA Chemical Engineering School announcement.
2023	Professor Honoris Causa of the University of West Attica, Department of Informatics and Computer Engineering; Award ceremony on 20 January 2023.
2022	The Best Oral Presentation Prize in the area "Processes and Systems Engineering and Control" at the 13th Panhellenic Scientific Conference in Chemical Engineering, 2-4 June 2022, to Paris Papavasileiou, PhD candidate. His presentation: "Assessment of CFD and ML modelling strategies for industrial-scale CVD reactors", by P. Papavasileiou, E. D. Koronaki, G. Pozzetti, M. Kathrein, C. Czettl, S. P. A. Bordas and A. G. Boudouvis.
2021	Elected Co-Chairman, Presidents Board, European University EULiST - European Universities Linking Society and Techology", 2021-2023.
2020	The *Léopold Escande 2019 Prize* for best doctoral theses of the Institut National Polytechnique de Toulouse (INPT), to Giorgos Gakis (thesis advisors A. G. Boudouvis and Prof. B. Caussat).
2017	Best NTUA Doctoral Thesis Award of the year 2012, by the Sarafis Foundation, to Nikos Cheimarios (thesis advisor A. G. Boudouvis).
2016	The *Léopold Escande 2016 Prize* for best doctoral theses of the Institut National Polytechnique de Toulouse (INPT), to Ioannis Aviziotis (thesis advisors A. G. Boudouvis, Dr. C. Vahlas and Dr. T. Duguet).
1995, 1999, 2004, 2008, 2009, 2010, 2011, 2012, 2013, 2015, 2016, 2017, 2019	Awards to diploma theses completed under A. G. Boudouvis' supervision: by the Technical Chamber of Greece (1995, 2004); by the Hellenic Society for Theoretical and Applied Mechanics (1999); by the National Technical University of Athens with the Thomaidis Foundation Distinction (2005); by the Thomaidis Foundation (NTUA) with the 3rd prize for Best Diploma Thesis of the year (2008); by the School of Chemical Engineering (2009, 2010, 2011, 2012, 2014, 2015, 2016, 2017, 2019); First Prize for Diploma thesis oral presentation at the 9th Panhellenic Conference in Chemical Engineering (2013).
2010	Best Doctoral Thesis Award of the year 2007, by the Thomaidis Foundation (NTUA), to Nikos Vourdas (thesis advisor A. G. Boudouvis).
1995	The 2nd Prize for best presentation in "Research and Technology Days '95", National Technical University of Athens
1984-1985	Doctoral Dissertation Fellowship, University of Minnesota
1979-1980	Fellowship, State Scholarship Foundation (IKY)
1976-1981	Fellowship, "I. S. Latsis" Foundation
1976	The First National Prize, Panhellenic Student Competition of the Hellenic Mathematical Society

MEMBER

Former: American Institute of Chemical Engineers, Society for Industrial and Applied Mathematics, American Mathematical Society.
European Community on Computational Methods in Applied Sciences (ECCOMAS), European Mechanics Society (EUROMECH), International Association for Computational Mechanics (IACM), Hellenic Mathematical Society,

Hellenic Society for Theoretical and Applied Mechanics, Greek Association of Computational Mechanics, Greek Association of Chemical Engineers, Technical Chamber of Greece.

PROFESSIONAL ACTIVITIES

a) Conference Organization *(recent/selected)*

- *Hellenic Institute of Advanced Studies Summer 2023 Events,* Athens, Greece, 3-7 July 2023. Member of the Organizing Committee.
- *14th European Fluid Mechanics Conference (EFMC14),* Athens, Greece, 13-16 September 2022. Member of the Local Organizing Committee.
- *Hellenic Institute of Advanced Studies Inaugural Symposium,* Athens, Greece, 8 July 2022. Member of the Organizing Committee.
- *45th International Conference on Micro & Nano Engineering (MNE 2019),* Rhodes, Greece, 23-26 September 2019. Member of the International Advisory Committee.
- *12th Hellenic Chemical Engineering Conference,* Athens, Greece, 29-31 May 2019. Member of the Scientific Committee.
- *The 6th European Conference on Computational Mechanics- ECCM 6 and the 7th European Conference on Computational Fluid Dynamics-ECFD 7,* Glasgow, UK, 11-15 June 2018. Member of the Scientific Committee.
- *9th GRACM International Congress on Computational Mechanics,* Chania, Greece, 4-6 June 2018. Member of the Organizing and Scientific Committee.
- *C-MAC Days 2017*, Athens, Greece, 20 - 23 November 2017. Chairman of the Organizing Committee.
- *1st International Conference on Computational Methods and Algorithms on HPC Platforms and Accelerators (CompHPC 2017),* Athens, Greece, 18 - 20 September 2017. Member of the Scientific Committee.
- *11th Hellenic Chemical Engineering Conference*, Thessaloniki, Greece, 25-27 May 2017. Member of the Scientific Committee.
- *12th World Congress on Computational Mechanics (WCCM XII) and 6th Asia-Pacific Congress on Computational Mechanics (APCOM VI) Congress 2016*, Seoul, Korea, 24-29 July 2016. Member of the International Scientific Committee.
- *European Congress on Computational Methods in Applied Sciences and Engineering (ECCOMAS) Congress 2016*, Chania, Crete Island, Greece, 5-10 June 2016. Member of the Local Organizing Committee and the Scientific Committee.
- *8th GRACM International Congress on Computational Mechanics*, Volos, Greece, 12-15 July 2015. Member of the Scientific Committee.
- *10th Hellenic Chemical Engineering Conference*, Patras, Greece, 4-6 June 2015. Member of the Organizing and Scientific Committees.
- *9th Pan-Hellenic Meeting on "Fluid Flow Phenomena"*, Athens, Greece, 12-13 December 2014. Member of the Organizing and the Scientific Committee.
- *Sixth Conference in Numerical Analysis (NumAn 2014): Recent Approaches to Numerical Analysis: Theory, Methods and Applications*, Chania, Crete, Greece, 2-5 September 2014. Member of the Scientific Committee.
- *11th World Congress on Computational Mechanics (WCCM XI),* Barcelona, Spain, 20-25 July 2014. Member of the International Scientific Committee.

b) Professional Service

- Reviewer in the following journals – indicative list: AIChE Journal; Applied Numerical Mathematics; Applied Surface Science; Biomicrofluidics; Chemical Engineering Journal; Chemical Engineering Science; Computational Mechanics; Computer Methods in Applied Mechanics and Engineering; Computers and Chemical Engineering; Fuzzy Sets and Systems; Industrial & Engineering Chemistry Research; International Journal for Numerical Methods in Fluids; International Journal of Heat and Mass Transfer; Journal of Applied Physics; Journal of Chemical Physics; Journal of Colloid and Interface Science; Journal of Computational Physics; Journal of Crystal

Growth; Journal of Fluid Mechanics; Journal of Food Science; Journal of Magnetism and Magnetic Materials; Journal of Materials Science; Journal of Membrane Science; Journal of Non-Newtonian Fluid Mechanics; Journal of Petroleum Science and Engineering; Journal of Physics: Condensed Matter; Journal of Physics D: Applied Physics; Langmuir; Materials Science in Semiconductor Processing; Microelectronic Engineering; Microfluidics and Nanofluidics; Parallel Computing; Physical Review E; Physical Review Letters; Physics of Fluids; Quarterly of Applied Mathematics; Sensors & Actuators: B. Chemical; Surface and Coatings Technology; Thin Solid Films.

- Reviewer of research proposals to the *United States Department of Energy,* USA
- Reviewer of research proposals to the *Agence Nationale de la Recherche*, France
- Reviewer of research proposals to the *Israel Science Foundation*, Israel
- Reviewer of research proposals to the *Technology Foundation STW*, The Netherlands
- Reviewer of research proposals to the *Qatar National Research Fund*, Qatar
- Reviewer of proposals to the *Leading Fellows Postdoc Programme*, Delft University of Technology, The Netherlands
- Reviewer of proposals to the *Cyprus Research Promotion Foundation*, Cyprus

- Member of the Executive Council, *Greek Association of Computational Mechanics*. 1995- President, 2007-2010
- Member of the Examinations Committee for Graduate Studies Scholarships, *State Scholarships Foundation*. 1996-2006
- Member of the International Council, *International Association for Hydromagnetic Phenomena and Applications*. 1996-2000
- Member of the Experts Committee for proposal evaluations for high-tech applications, *General Secretariat for Research and Technology*. 1997-present
- Member of the Experts Committee for proposal evaluations for the "Human Networks for R&D" Program, *General Secretariat for Research and Technology*. 1999
- Member of the Executive Council, *Scientific & Educational Center of Chemical Engineers S.A.* 2000-2006
- Member of the Management Committee, *Program COST*, Action P6 of the European Commission. 2000-05
- Member of the Computational Fluid Dynamics Committee, *European Community on Computational Methods in Applied Sciences (ECCOMAS)*. 2001-present
- Member of the General Council, *International Association for Computational Mechanics (IACM).* 2009-present
- Member of the Management Committee, *Program COST*, Action P17 of the European Commission. 2005-2009

c) Institutional Service *(selected)*

- *General Assembly*, School of Chemical Engineering, NTUA. Member, 1993-94, 1997-98, 1999-present.
- *Senate*, NTUA. 1993-94, 1997-98, 2013-2016, 2019-2023
- *Management Committee* for the funds of the 2nd Community Support Framework, School of Chemical Engineering, NTUA. Coordinator, 1995-99.
- *Institutional Committee* for the Student Exchange Program Erasmus/Socrates, NTUA. Member, 1996-2000.
- *Panel* for the "Self-Evaluation of the Education and Services provided by the National Technical University of Athens", NTUA. Member, 1997-1999.
- *Supercomputing Committee*, NTUA. Member, 1997-2001.
- *Executive Committee* of the Inter-Departmental Postgraduate Program "Mathematical Modeling in Modern Technologies and Financial Engineering", NTUA. Member, 2003-2018.
- *Executive Committee* of the Inter-Departmental Graduate Studies Program "Computational Mechanics", NTUA. Member, 2005-present and Director, 2011-2018.

RESEARCH PUBLICATIONS

- 154 publications in peer-reviewed international journals
- More than 150 publications and presentations at international conferences

PUBLICATIONS, 2015-present

In journals (2015 – present; numbering starts from 97)

154. G. P. Gakis, G. L. Suntaxi, I. G. Aviziotis, E. D. Koronaki, P. P. Filippatos, G. Chatzigiannakis, S.P.A. Bordas, D. Davazoglou and A. G. Boudouvis "CFD modelling and sensitivity-guided design of Silicon filament CVD reactors." *AIChE J.* **e70428** (2026).

153. D. Angelidis, N. Cheimarios and A. G. Boudouvis "Computational investigation of the Kelvin-Helmholtz instability: From Thorpe's experiment to reactive flows." *Meccanica* **61:50** (2026).

152. E. D. Koronaki, D. G. Giovanis, G. L. Suntaxi, M. Kathrein, C. Czettl, A. G. Boudouvis and S.P.A. Bordas "From data to process insights: Hybrid modeling strategies for chemical vapor deposition processes." *International Journal of Refractory Metals and Hard Materials* **138**, 107750 (2026).

151. A. Lazou, G. P. Gakis, D. Marinos, I. G. Aviziotis, E. Balomenos, A. G. Boudouvis and D. Panias "CO_2 absorption in NaOH-Na_2CO_3 solutions: Combined CFD and thermodynamics-based, experimentally validated analysis." *Chemical Engineering Science* **327**, 123613 (2026).

150. E. D. Koronaki, G. L. Suntaxi, P. Papavasileiou, D. G. Giovanis, M. Kathrein, C. Czettl, A. G. Boudouvis and S.P.A. Bordas "Implementing NLPs in industrial process modeling: Addressing categorical variables." *Computers and Chemical Engineering* **199**, Art. 109146 (2025).

149. G. P. Gakis, D. Marinos, I.G. Aviziotis, E. Balomenos, A.G. Boudouvis and D. Panias "An integrated, CFD-based, analysis of carbonation in a stirred tank reactor." *Materials* **18**, 1535 (2025).

148. A. Papavasileiou, D. G. Giovanis, G. Pozzetti, M. Kathrein, C. Czettle, I. G. Kevrekidis, A. G. Boudouvis, S.P.A. Bordas and E. D. Koronaki "Integrating supervised and unsupervised learning approaches to unveil critical process inputs." *Computers and Chemical Engineering* **192**, Art. 108857 (2025).

147. G. L. Suntaxi, P. Papavasileiou, E. D. Koronaki, D. G. Giovanis, G. P. Gakis, I. G. Aviziotis, M. Kathrein, G. Pozzetti, C. Czettle, S.P.A. Bordas and A. G. Boudouvis "Discovering deposition process regimes: Leveraging unsupervised learning for process insights, surrogate modeling, and sensitivity analysis." *Chemical Engineering Journal Advances* **20**, Art. 100667 (2024).

146. A. G. Koulidis, A. G. Progiou, I. Sebos and A. G. Boudouvis "Exploring input parameter effects on air pollution dispersion models: Uncertainty and implications for environmental assessments." *Environmental Engineering and Management Journal* **23**, 2221 (2024).

145. A. P. Papavasileiou, E. D. Koronaki, G. Pozzetti, M. Kathrein, C. Czettl, A. G. Boudouvis and S.P.A. Bordas "Equation-based and data-driven modeling strategies for industrial coating processes." *Computers in Industry* **149**, 103938 (2023).

144. E. D. Koronaki, N. Evangelou, Y. M. Psarellis, A. G. Boudouvis and I. G. Kevrekidis "From partial data to out-of-sample parameter and observation estimation with Diffusion Maps and Geometric Harmonics." *Computers and Chemical Engineering* **178**, Art. 108357 (2023).

143. P. Papavasileiou, E. D. Koronaki, G. Pozzetti, M. Kathrein, C. Czettl, A. G. Boudouvis, T.J. Mountziaris, S.P.A. Bordas "An efficient chemistry-enhanced CFD model for the investigation of the rate-limiting mechanisms in industrial Chemical Vapor Deposition reactors." *Chemical Engineering Research and Design* **186**, 314 (2022).

142. A. S. Mouchtouris, G. Kokkoris and A. G. Boudouvis "Predicting power-voltage characteristics and mode transitions in the COST reference microplasma jet." *Journal of Physics D: Applied Physics* **55**, 355203 (2022).

141. M. Kavousanakis, N. Cheimarios, G. Kokkoris and A. G. Boudouvis "On the effect of self-sustained periodic flows on film thickness non-uniformity during CVD." *Computers and Chemical Engineering* **161**, Art. 107775 (2022).

140. A. Fytopoulos, M. Kavousanakis, T. Van Gerven, A. G. Boudouvis, G. Stefanidis and C. Xiouras "Crystal growth, dissolution and agglomeration kinetics of Sodium Chlorate." *Industrial & Engineering Chemistry Research* **60**, 7367 (2021).

139. N. Cheimarios, D. To, G. Kokkoris, G. Memos and A. G. Boudouvis "Monte Carlo & Kinetic Monte Carlo models for deposition processes: A review of recent works." *Frontiers in Physics* **9**, Art. 631918 (2021).

138. R. Spencer, P. Gkinis, E. D. Koronaki, D. I. Gerogiorgis, S. P. A. Bordas and A. G. Boudouvis "Investigation of the chemical vapor deposition of Cu from copper amidinate through data driven efficient CFD modelling." *Computers and Chemical Engineering* **149**, Art. 107289 (2021).

137. A. Hadjigeorgiou, A. G. Boudouvis and G. Kokkoris "Thorough computational analysis of the staggered herringbone mixer reveals transport mechanisms and enables mixing efficiency-based improved design." *Chemical Engineering Journal* **414**, Art. 128775 (2021).

136. T. N. Papapetrou, G. Lecrivain, M. Bieberle, A. G. Boudouvis and U. Hampel "An improved contact method for quantifying the mixing of a binary granular mixture." *Granular Matter* **23** Art. 15 (2021).

135. N. Cheimarios, G. Kokkoris and A. G. Boudouvis "Multiscale modeling in chemical vapor deposition processes: Models and methodologies." *Archives of Computational Methods in Engineering* **28**, 637 (2021)

134. E. D. Koronaki, A. M. Nikas and A. G. Boudouvis "A data-driven reduced-order model of nonlinear processes based on Diffusion Maps and Artificial Neural Networks." *Chemical Engineering Journal* **397**, 125475 (2020).

133. A. Dafnomilis, S. Diab, A. Rodman, A. G. Boudouvis and D. I. Gerogiorgis "Multi-objective dynamic optimization of ampicillin batch crystallization: Sensitivity analysis of attainable performance vs. product quality constraints." *Industrial & Engineering Chemistry Research* **58** (40) 18756 (2019).

132. G. P. Gakis, H. Vergnes, F. Cristiano, Y. Tison, C. Vahlas, B. Caussat, A. G. Boudouvis and E. Scheid "In situ N_2-NH_3 plasma pre-treatment of silicon substrate enhances the initial growth and restricts the substrate oxidation during alumina ALD." *Journal of Applied Physics* **126**, 125305 (2019).

131. D. Lentzou, A. G. Boudouvis, V. Karathanos and G. Xanthopoulos "A moving boundary model for fruit isothermal drying and shrinkage: An optimisation method for water diffusivity and peel resistance estimation." *Journal of Food Engineering* **263**, 299 (2019).

130. G. P. Gakis, C. Vahlas, H. Vergnes, S. Dourdain, Y. Tison, H. Martinez, J. Bour, D. Ruch, A. G. Boudouvis, B. Caussat and E. Scheid "Investigation of the initial deposition steps and the interfacial layer of Atomic Layer Deposited (ALD) Al_2O_3 on Si." *Applied Surface Science* **492**, 245 (2019).

129. N. Vourdas, G. Pashos, G. Kokkoris, E. Rizos, L. Tsampasis, E. Klouvidaki, A. G. Boudouvis and V. Stathopoulos "Plug actuation and active manipulation in closed monolithic fluidics using backpressure." *Microelectronic Engineering* **216**, 111046 (2019).

128. V. Krokos, G. Pashos, A. N. Spyropoulos, G. Kokkoris, A. G. Papathanasiou and A. G. Boudouvis "Optimization of patterned surfaces for improved superhydrophobicity through cost-effective large-scale computations." *Langmuir* **35**, 6793 (2019).

127. A. N. Spyropoulos, A. G. Papathanasiou and A. G. Boudouvis "2-3-4 spikes competition in the Rosensweig instability." *Journal of Fluid Mechanics* **870**, 389 (2019).

126. G. Xanthopoulos, A. Athanasiou, A. Sempou, D. Lentzou, Ch. Templalexis and A. G. Boudouvis "Study of the drying rate and colour kinetics during stepwise air-drying of apricot halves." *International Journal of Food Engineering* **15**, 20180372 (2019).

125. N. Cheimarios, M. E. Kavousanakis, G. Kokkoris and A. G. Boudouvis "Beware of symmetry breaking and periodic flow regimes in axisymmetric CVD reactor setups." *Computers & Chemical Engineering* **124**, 124 (2019).

124. P. A. Gkinis, E. D. Koronaki, A. Skouteris, I. G. Aviziotis and A. G. Boudouvis "Building a data-driven Reduced Order Model of a Chemical Vapor Deposition process from low-fidelity CFD simulations." *Chemical Engineering Science* **199**, 371 (2019).

123. S. Diab, N. Mytis, A. G. Boudouvis and D. I. Gerogiorgis "Process modelling, design and technoeconomic liquid-liquid extraction (LLE) optimisation for comparative evaluation of batch vs. continuous pharmaceutical manufacturing of atropine." *Computers & Chemical Engineering* **124**, 28 (2019).

122. E. D. Koronaki, P.A. Gkinis, L. Beex, S.P.A. Bordas, C. Theodoropoulos and A. G. Boudouvis "Classification of states and model order reduction of large scale Chemical Vapor Deposition processes with solution multiplicity." *Computers & Chemical Engineering* **121**, 148 (2019).

121. G. P. Gakis, H. Vergnes, E. Scheid, C. Vahlas, A. G. Boudouvis and B. Caussat "Detailed investigation of the surface mechanisms and their interplay with transport phenomena in alumina atomic layer deposition from TMA and water." *Chemical Engineering Science* **195**, 399 (2019).

120. P. Chrysinas, G. Pashos, N. Vourdas, G. Kokkoris, V. Stathopoulos and A. G. Boudouvis "Investigation of actuation mechanisms of droplets on porous air-permeable substrates." *Soft Matter* **14**, 6090 (2018).

119. C. Xiouras, A. A. Fytopoulos, J. H. Ter Horst, A. G. Boudouvis, T. Van Gerven and G. D. Stefanidis "Particle breakage kinetics and mechanisms in attrition-enhanced deracemization." *Crystal Growth & Design* **18**, 3051 (2018).

118. G. P. Gakis, H. Vergnes, E. Scheid, C. Vahlas, B. Caussat and A. G. Boudouvis "Computational Fluid Dynamics simulation of the ALD of alumina from TMA and H_2O in a commercial reactor." *Chemical Engineering Research and Design* **132**, 795 (2018).

117. C. Xiouras, A. Fytopoulos, J. Jordens, A. G. Boudouvis, T. Van Gerven and G. Stefanidis “Application of ultrasound to chiral crystallization, resolution and deracemization." *Ultrasonics Sonochemistry* **43**, 184 (2018).

116. P. Chrysinas, M. E. Kavousanakis and A. G. Boudouvis "Effect of cell heterogeneity on isogenic populations with the synthetic genetic toggle switch network: bifurcation analysis of two dimensional Cell Population Balance Models." *Computers & Chemical Engineering* **112**, 27 (2018).

115. I. Michalopoulos, T. Kamperidis, G. Seintis, G. Pashos, C. Lytras, K. Papadopoulou, A. G. Boudouvis and G. Lyberatos “Experimental and numerical assessment of the hydraulic behavior of a pilot-scale periodic anaerobic baffled reactor (PABR)." *Computers & Chemical Engineering* **111**, 278 (2018).

114. G. Psarellis, I. G. Aviziotis, T. Duguet, C. Vahlas, E. D. Koronaki and A. G. Boudouvis "Investigation of reaction mechanisms in the chemical vapor deposition of Al from DMEAA." *Chemical Engineering Science* **177**, 464 (2018).

113. I. G. Aviziotis, T. Duguet, K. Soussi, M. Heggen, M.-C. Lafont, F. Morfin, S. Mishra, S. Daniele, A. G. Boudouvis and C. Vahlas "Chemical Vapor Deposition of approximant m-$Al_{13}Fe_4$ films for the catalytic semi-hydrogenation of acetylene." *Physica Status Solidi A* **215***,* 1700692 (2018).

112. I. G. Aviziotis, T. Duguet, C. Vahlas and A. G. Boudouvis "Combined macro-/nano-scale investigation of the CVD of Fe from $Fe(CO)_5$." *Advanced Materials Interfaces* **4**, 1601185 (2017).

111. N. M. Dimitriou, G. Tsekenis, E. C. Balanikas, A. Pavlopoulou, M. Mitsiogianni, T. Mantso, G. Pashos, A. G. Boudouvis, I. N. Lykakis, G. Tsigaridas, M. I. Panayiotidis, V. Yannopapas and A. G. Georgakilas "Gold nanoparticles, radiations and the immune system: Current insights into the physical mechanisms and the biological interactions of this new alliance towards cancer therapy." *Pharmacology & Therapeutics* **178**, 1 (2017).

110. P. A. Gkinis, I. G. Aviziotis, E. D. Koronaki, G. P. Gakis and A. G. Boudouvis "The effects of flow multiplicity on GaN deposition in a rotating disk CVD reactor." *Journal of Crystal Growth* **458**, 140 (2017).

109. A. Papadopoulos, T. Tsoutsos, M. Frangou, K. Kalaitzakis, N. Stefanakis and A. G. Boudouvis "Innovative optics for concentrating photovoltaic/thermal (CPVT) systems - The case of Proteas solar polygeneration system." *International Journal of Sustainable Energy* **36**, 775 (2016).

108. A. K. Karalis, N. Karkalos, N. Cheimarios, G. Antipas, A. Xenidis and A. G. Boudouvis “A CFD analysis of slag properties, electrode shape and immersion depth effects on electric submerged arc furnace heating in ferronickel processing.” *Applied Mathematical Modelling* **40**, 9052 (2016).

107. I. G. Aviziotis, N. Cheimarios, T. Duguet, C. Vahlas and A. G. Boudouvis "Multiscale modeling and experimental analysis of chemical vapor deposited aluminum films: linking reactor operating conditions with roughness evolution." *Chemical Engineering Science* **155**, 449 (2016).

106. N. Cheimarios, G. Kokkoris and A. G. Boudouvis "A multi-parallel multiscale computational framework for chemical vapor deposition processes." *Journal of Computational Science* **15**, 81 (2016).

105. N. Vourdas, G. Pashos, G. Kokkoris, A. G. Boudouvis and V. N. Stathopoulos "Droplet mobility manipulation on porous media using backpressure." *Langmuir* **32**, 5250 (2016).

104. E. D. Koronaki , G. P. Gakis, N. Cheimarios and A. G. Boudouvis "Efficient tracing and stability analysis of multiple stationary and periodic states with exploitation of commercial CFD software." *Chemical Engineering Science* **150**, 26 (2016).

103. G. N. Chamakos, M. E. Kavousanakis, A. G. Boudouvis and A. G. Papathanasiou "Droplet spreading on rough surfaces: tackling the contact line boundary condition." *Physics of Fluids* **28**, 022105 (2016).

102. G. Pashos, G. Kokkoris, A. G. Papathanasiou and A. G. Boudouvis "Wetting transitions on patterned surfaces with diffuse interaction potentials embedded in a Young-Laplace formulation." *Journal of Chemical Physics* **144**, 034105 (2016).

101. G. P. Gakis, E. D. Koronaki and A. G. Boudouvis "Numerical investigation of multiple stationary and time-periodic flow regimes in vertical rotating disk CVD reactors." *Journal of Crystal Growth* **432**, 152-159 (2015).

100. G. Pashos, G. Kokkoris and A. G. Boudouvis "Minimum energy paths of wetting transitions on grooved surfaces." *Langmuir* **31**, 3059 (2015).

99. I. G. Aviziotis, M. E. Kavousanakis and A. G. Boudouvis "Effect of intrinsic noise on the phenotype of cell populations featuring solution multiplicity: an artificial lac operon network paradigm." *PLOS ONE* **10**(7), e0132946 (2015).

98. I. G. Aviziotis, M. E. Kavousanakis, I. A. Bitsanis and A. G. Boudouvis "Coarse-grained analysis of stochastically simulated cell populations with a positive feedback genetic network architecture." *Journal of Mathematical Biology* **70**, 1457 (2015).

97. G. Pashos, G. Kokkoris and A. G. Boudouvis "A modified phase-field method for the investigation of wetting transitions of droplets on patterned surfaces." *Journal of Computational Physics* **283**, 258 (2015).

Selected conference presentations (2015 – present; numbering starts from 78)

105. A. Smolla, A. G. Sourais, S. S. Kantorovich, A. G. Boudouvis and R. Richter "Force enhancement in-between suszeptible dipolar hard spheres- measurement vs computation." *2025 Deutsche Physikalische Gesellschaft (DPG) Spring Meeting*, Regensburg, Germany, 16-21 March 2025.

104. G. Loachamín, P. Papavasileiou, E. Koronaki, D. Giovanis, I. Aviziotis, G. Gakis, G. Pozzetti, M. Kathrein, C. Czettl, A. Boudouvis and S. Bordas "Navigating Chemical Vapour Deposition regimes: Leveraging Unsupervised Learning for process insights, surrogate modeling, and sensitivity analysis." *2024 ECCOMAS Congress*, Lisbon, Portugal, 3-7 June 2024.

103. P. Papavasileiou, E. D. Koronaki, D. G. Giovanis, G. Pozzetti, M. Kathrein, C. Czettl, A. G. Boudouvis and S. P. A. Bordas, "Investigation of defining process inputs using unsupervised machine learning." *14th European Congress of Chemical Engineering and 7th European Congress of Applied Biotechnology*, Berlin, Germany, 17-21 September 2023.

102. P. Papavasileiou, E. D. Koronaki, G. Pozzetti, M. Kathrein, C. Czettl, A. G. Boudouvis and S. P. A. Bordas, "An efficient CFD model of an industrial scale CVD reactor allowing accurate coating thickness predictions." *WCCM-APCOM 15th Virtual World Congress on Computational Mechanics and 8th Asian Pacific Congress on Computational Mechanics*, Yokohama, Japan, 31 July-5 August 2022.

101. P. Papavasileiou, E. D. Koronaki, G. Pozzetti, M. Kathrein, C. Czettl, A. G. Boudouvis and S. P. A. Bordas, "A comparison of equation-based and machine learning models of industrial scale deposition processes." *ECCOMAS 2022 International Congress on Computational Mechanics*, Oslo, Norway, 5-9 June 2022.

100. E. D. Koronaki, N. Evangelou, Y. Psarellis, A. G. Boudouvis and I. G. Kevrekidis "From partial data to out-of-sample parameter and observation estimation with Diffusion Maps and Geometric Harmonics." *2020 Virtual AIChE Annual Meeting*, 16-20 November 2020.

99. G. P. Gakis, H. Vergnes, F. Cristiano, C. Vahlas, B. Caussat, A. G. Boudouvis and E. Scheid "Reduction of the growth inhibition and substrate oxidation during the first steps of alumina ALD on Si by an *in situ* N_2-NH_3 plasma surface pre-treatment." *5th Réseau des Acteurs Français de l' Atomic Layer Deposition (RAFALD)*, Toulouse, France, 5-7 November 2019.

98. E. D. Koronaki, P. A. Gkinis and A. G. Boudouvis "A Reduced Order Modelling framework for CVD processes based on low-fidelity data." *Joint 22nd European Chemical Vapor Deposition & 16th Baltic Atomic Layer Deposition Conference (Euro CVD 22 – Baltic ALD 16)*, Luxembourg, 24-28 June 2019.

97. D. Davazoglou, K. Peloriadou, G. Papadimitropoulos, N. Vourdas, A. Soultati, M. Vasilopoulou, I. G. Aviziotis and A. G. Boudouvis "Chemical vapor deposition of Tin and of Erbium oxide and Er-doped SnO_2 films." *Joint 22nd European Chemical Vapor Deposition & 16th Baltic Atomic Layer Deposition Conference (Euro CVD 22 – Baltic ALD 16)*, Luxembourg, 24-28 June 2019.

96. A. N. Spyropoulos, A. G. Papathanasiou and A. G. Boudouvis "2-3-4 spikes competition in the normal field instability of ferrofluids." *9th International Meeting of the Hellenic Society of Rheology*, Pythagorion, Samos, Greece, 23-27 June 2019.

95. P. A. Gkinis, E. D. Koronaki and A. G. Boudouvis "Reduced order modeling of reactive transport: application in CVD processes." *ECMetAC Days 2018*, Poznan, Poland, 3-5 December 2018.

94. G.P. Gakis, H. Vergnes, E. Scheid, C. Vahlas, A. G. Boudouvis and B. Caussat "Initial growth of Alumina ALD: Effect of substrate pretreatment on nucleation period reduction. A computational mechanistic investigation." *4th Réseau des Acteurs Français de l' Atomic Layer Deposition (RAFALD),* Lyon, France, 6-8 November 2018.

93. G.P. Gakis, H. Vergnes, E. Scheid, C. Vahlas, A. G. Boudouvis and B. Caussat "Alumina ALD from TMA and Water: Unravelling the surface mechanisms and linking transport phenomena with growth uniformity." *2018 Fall Meeting of the European Materials Research Society (EMRS),* Warsaw, Poland, 17-20 September 2018.

92. A. A. Fytopoulos, C. Xiouras, M.E. Kavousanakis, T. Van Gerven, A. G. Boudouvis and G. D. Stefanidis "A population balance model for temperature cycling-enhanced deracemization." *25th International Workshop on Industrial Crystallization (BIWIC)*, Rouen, France, 5-7 September 2018.

91. P. A. Gkinis, A. Skouteris, E. D. Koronaki and A. G. Boudouvis "A reduced-order model for efficient CFD analysis of Chemical Vapor Deposition processes." *9th GRACM International Congress on Computational Mechanics*, Chania, Crete, Greece, 4-6 June 2018.

90. G.P. Gakis, H. Vergnes, E. Scheid, C. Vahlas, B. Caussat and A. G. Boudouvis "Experimental investigation and CFD-based analysis of an ALD reactor depositing alumina from TMA and water." *3rd Réseau des Acteurs*

Français de l' Atomic Layer Deposition (RAFALD), Montpellier, France, 7-9 November 2017.

89. I. G. Aviziotis, T. Duguet, C. Vahlas and A. G. Boudouvis "Multiscale analysis of reactive transport processes: A tool to monitor the microstructure and the properties of chemical vapor deposited films." *EUROMAT 2017*, Thessaloniki, Greece, 17-22 September 2017.

88. G.P. Gakis, H. Vergnes, E. Scheid, A. G. Boudouvis, C. Vahlas and B. Caussat "Experimental investigation and CFD-based analysis of an ALD reactor depositing alumina from TMA and water." *Joint 21st European Chemical Vapor Deposition & 15th Baltic Atomic Layer Deposition Conference (EuroCVD 21 – Baltic ALD 15)*, Linköping, Sweden, 11 – 14 June 2017.

87. I. G. Aviziotis, T. Duguet, C. Vahlas and A. G. Boudouvis "Chemical vapor deposition of Al, Fe and of the $Al_{13}Fe_4$ approximant intermetallic phase: Experiments and multiscale simulations." *C-MAC Days 2016*, Bratislava, Slovakia, 21-23 November 2016.

86. G.P. Gakis, H. Vergnes, E. Scheid, A. G. Boudouvis, C. Vahlas and B. Caussat "CFD analysis of an ALD reactor: gaseous species distribution and cycle time." *2nd Réseau des Acteurs Français de l' Atomic Layer Deposition (RAFALD),* Chatou/Paris, France, 14-16 November 2016.

85. I. G. Aviziotis, T. Duguet, A. G. Boudouvis and C. Vahlas "$Al_{13}Fe_4$ intermetallic coatings processed by chemical vapor deposition." *13th International Conference on Nanoscience and Nanotechnologies (NN16)*, Thessaloniki, Greece, 5-8 July 2016.

84. G. Kasapidis, G. Pashos, G. Kokkoris and A.G. Boudouvis "Fast computations on GPUs for wetting phenomena." *The European Community on Computational Methods in Applied Sciences (ECCOMAS) Congress 2016,* Chania, Crete Island, Greece, 5-10 June 2016.

83. G. Pashos, G. Kokkoris and A.G. Boudouvis "Computations of wetting transitions on grooved surfaces." *11th Hellenic Society for Theoretical and Applied Mechanics (HSTAM) International Congress on Mechanics,* Athens, Greece, 27-30 May 2016.

82. I. G. Aviziotis, T. Duguet, A. G. Boudouvis and C. Vahlas "$Al_{13}Fe_4$ coatings obtained by chemical vapor deposition." *International Conference on Metallurgical Coatings and Thin Films (ICMCTF),* San Diego, USA, 25-29 April 2016.

81. G. Pashos, G. Kokkoris and A. G. Boudouvis "Computation of wetting states on patterned surfaces with a modified phase-field method." *8th GRACM International Congress on Computational Mechanics*, Volos, Greece, 12-15 July 2015.

80. P. I. Giannatselis, N. Cheimarios , E. D. Koronaki and A. G. Boudouvis "Tracing axisymmetric and non axisymmetric states in chemical vapor deposition reactors." *8th GRACM International Congress on Computational Mechanics*, Volos, Greece, 12-15 July 2015.

79. G. Pashos, G. Kokkoris and A. G. Boudouvis "Fast computations of wetting transitions on GPUs." *International Computational Science and Engineering Conference (ICSEC15)*, Doha, Qatar, 11-12, May 2015.

78. N. Cheimarios, G. Kokkoris and A. G. Boudouvis "Multiscale analysis of reactive transport in thin film deposition processes." *International Computational Science and Engineering Conference (ICSEC15)*, Doha, Qatar, 11-12, May 2015.