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Polymer Reaction Engineering XI

Proceedings

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Program

Polymer Reaction Engineering XI

December 11 - 15, 2022 The Scottsdale Plaza Resort Scottsdale, Arizona, USA

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Conference Co-Chair

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Engineering Conferences International (ECI) is a not-for-profit global engineering conferences program, originally established in 1962, that provides opportunities for the exploration of problems and issues of concern to engineers and scientists from many disciplines.

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Polymer Reaction Engineering March 10-15, 1991 Santa Barbara, California Conference Chairs:

Charles Cozewith, Exxon Chemical, USA Charles Barren, Clemson University, USA

Polymer Reaction Engineering II February 13-18, 1994 Palm Coast, Florida Conference Chairs:

Eugene P. Dougherty, Rohm & Haas, USA Joseph Schork, Georgia Institute of Technology, USA

Polymer Reaction Engineering III March 16-21, 1997 Palm Coast, Florida

Conference Chairs: Kyu Yung Choi, University of Maryland, USA Dr. Michael E. Muhle, Exxon Chemical, USA Michael Cunningham, Xerox, USA

Polymer Reaction Engineering IV March 19-24, 2000 Palm Coast, Florida

Conference Chairs: Michael Cunningham, Queens University, Canada K.W. Leffew, DuPont Central R&D, USA K.B. McAuley, Queens University, Canada

Polymer Reaction Engineering V May 18-23, 2003 Quebec City, Canada Conference Chairs:

Joao B.P. Soares, University of Waterloo, Canada Rafael Galvan, Johnson Polymer, UK Robin A. Hutchinson, Queen's University, Canada

Polymer Reaction Engineering VI May 21-26, 2006 Halifax, Nova Scotia, Canada

Conference Chairs: Robin A. Hutchinson, Queen's University, Canada Michael Muhle, ExxonMobil Chemical Co., USA Alexander Penlidis, University of Waterloo, Canada

Previous conferences in this series:

Polymer Reaction Engineering VII May 3-8, 2009 Niagara Falls, Ontario, Canada *Conference Chairs:* Alexander Penlidis, University of Waterloo, Canada John R. Richards, DuPont, USA Marc A. Dube, University of Ottawa, Canada

Polymer Reaction Engineering VIII May 6-11, 2012 Cancun, Mexico

Conference Chairs: Marc A. Dube, University of Ottawa, Canada Marco Villalobos, Cabot Corp., USA Eduardo Vivaldo-Lima, UNAM, Mexico

Polymer Reaction Engineering IX May 10-15, 2015 Cancun, Mexico

Conference Chairs: Eduardo Vivaldo-Lima, UNAM, Mexico Jon Debling, BASF, USA Fernando Zaldo-Garcia, COMEX, Mexico John Tsavalas, University of New Hampshire, USA

Polymer Reaction Engineering X May 20 – May 25, 2018 Punta Cana, Dominican Republic Conference Chairs:

John Tsavalas, University of New Hampshire, USA Fouad Teymour, Illinois Institute of Technology, USA Jose R. Leiza, University of the Basque Country, Spain Jeffrey Stubbs, HP Inc., USA

Conference Sponsor

ExxonMobil Technology and Engineering Company

Sunday, December 11, 2022

| 16:30 – 18:00 | Conference check-in and Installation of Posters |
|---------------|--|
| 18:00 | Welcome reception followed by dinner (Cypress Court) |

Locations and Notes

- Technical sessions will be in Grand Ballroom C. Poster sessions will be in Grand Ballroom A/B.
- Meals will be in Grand Ballroom E/F.
- The ECI office is in Cactus A.
- Please wear your mask except when giving a presentation or actively eating or drinking. Please maintain physical distancing as much as possible.
- Audio, still photo and video recording by any device (e.g., cameras, cell phones, laptops, PDAs, watches) is strictly prohibited during the technical sessions, unless the author and ECI have granted prior permission.
- Speakers Please have your presentation loaded onto the conference computer prior to the session start (preferably the day before).
- Speakers Please leave at least 3-5 minutes for questions and discussion.
- Please do not smoke at any conference functions.
- Turn your mobile telephones to vibrate or off during technical sessions.
- After the conference, ECI will send an updated participant list to all participants. Please check your listing now and if it needs updating, you may correct it at any time by logging into your ECI account.
- Emergency Contact Information: Because of privacy concerns, ECI does not collect or maintain emergency contact information for conference participants. If you would like to have this information available in case of emergency, please use the reverse side of your name badge.

Monday, December 12, 2022

| Breakfast |
|--|
| Topic 1 |
| Developing strategies for polymer redesign and recycling using reaction pathway analysis Linda Broadbelt, Northwestern University, USA |
| Renewable barrier polymers from carbohydrates Carson Meredith, Georgia Tech, USA |
| |

- 10:30 11:00 Coffee break
- 11:00 11:30 Chemical recycling of polyethylene by tandem catalytic conversion to propylene Ivan Konstantinov, The Dow Chemical Company, USA
- 11:30 12:00Kinetic phenomena in mechanochemical depolymerization of poly(styrene)
George Y. Chang, Georgia Institute of Technology, USA
- 12:00 12:30 Ring-chain equilibrium for polyester recycling Flavio Tollini, Politecnico di Milano, Italy
- 12:30 14:00 Lunch

Topic 2

- 14:00 14:45 **Mathematical modeling for control of emulsion polymerization** Jose Maria Asua, POLYMAT, University of the Basque Country, Spain
- 14:45 15:15 Inline and offline particle size analysis in emulsion polymerization processes Usue Olatz Aspiazu, POLYMAT, Spain
- 15:15 15:45 **Performance analysis of kinetic Monte Carlo algorithms for synthesis of linear polymers** Alessandro D. Trigilio, Ghent University, Belgium
- 15:45 16:15Pushing forward the predictive power of kinetic Monte Carlo simulations
for detailed (de)polymerization chemistries
Yoshi W. Marien, Ghent University, Belgium
- 16:15 18:00 Posters / Social Hour / Networking
- 18:00 19:30 Dinner

Tuesday, December 13, 2022

| 08:00 - 09:00 | Breakfast |
|---------------|---|
| | Topic 2 (continued) |
| 09:00 – 09:45 | Process analytics with OptoFluidic Force Induction (OF2i). A BRAVE new way in online particle characterization Christian Hill, Medizinische Universität Graz, Austria |
| 09:45 – 10:30 | Industrial Acrylic Polymerization Modeling Michael Grady, Axalta, USA |
| 10:30 – 11:00 | Coffee break |
| 11:00 – 11:45 | How increasingly powerful PRE modeling tools allow to unlock the full potential of FRP and RDRP in aqueous emulsion Yoshi W. Marien, Ghent University, Belgium |
| 11:45 – 12:15 | Enforcing the formation of cycles in the random graph modelling of polymerising HDDA Tamika van 't Hoff, University of Amsterdam, the Netherlands |
| 12:15 – 14:00 | Lunch |
| | Topic 3 |
| 14:00 – 14:45 | A thermodynamic perspective on the medium dependence of propagation coefficients and reactivity ratios in radical polymerization Hugo Vale, BASF, Germany |
| 14:45 – 15:15 | Modelling of a multizone circulating reactor for propylene polymerization: Impact of thermodynamic model Kusuma Kulajanpeng, Université Claude Bernard Lyon 1, France |
| 15:15 – 15:45 | Mathematical modeling for 1,6-hexanediol diacrylate photopolymerization in presence of oxygen Kim McAuley, Queen's University, Canada |
| 15:45 – 16:15 | The use of high-temperature semi-batch radical polymerization to synthesize acrylate based macromonomers and structured copolymer dispersants Elizabeth Bygott, Queen's University, Canada |
| 16:15 – 16:45 | Understanding the microstructure differences in the emulsion polymerization of bio-based and oil-based C8 alkyl (meth)acrylates Aitor Barquero, UPV/EHU, Spain |
| 16:45 – 18:00 | Social Hour / Networking |
| 18:00 – 19:30 | Banquet |

Wednesday, December 14, 2022

| 08:00 - 09:00 | Breakfast |
|---------------|--|
| | Topic 3 (continued) |
| 09:00 – 09:45 | It's all about diffusion: Measurements and modeling of particle morphologies in dispersed-phase polymerization John Tsavalas, University of New Hampshire, USA |
| 09:45 – 10:30 | Understanding polymerization processes in detail by combining experimental and modeling studies Kristina Zentel, TU Darmstadt, Germany |
| 10:30 – 11:00 | Coffee break |
| 11:00 – 11:45 | Monomer transport limitations in emulsion polymerization Francis J. Schork, Georgia Tech, USA |
| | Topic 4 |
| 11:45 – 12:15 | Chemical and optical mixing characterization of a dynamic inline mixer Wladislaw Dolshanskiy, University of Hamburg, Germany |
| 12:15 – 14:00 | Lunch |
| 14:00 – 14:30 | Disentangled UHMWPE - Control of crystallization, chain entanglement and rheology via process conditions Roberta Lopes do Rosario, CP2M Lyon, France |
| 14:30 – 15:00 | Wall layer formation in continuously operated tubular reactors for free- radical polymerizations Stefan Welzel, University of Stuttgart, Germany |
| 15:00 – 15:30 | Reactive molding of elastomeres in 3D-printed molds for robotic actuators Alexey Stepanyuk, University of Hamburg, Germany |
| 15:30 - 18:00 | Social Hour / Networking |
| 18:00 – 19:30 | Dinner |

Thursday, December 15, 2022

08:00 Breakfast & Departures

Poster Presentations

- 1. **Mass transfer and agitation in the emulsion of PVDF** Timothy McKenna, CP2M UMR 5128, France
- 2. Mass transfer phenomena in vinylidene fluoride emulsion polymerization Timothy McKenna, CP2M UMR 5128, France
- 3. Gas phase ethylene polymerization: What is the influence of condensed mode Timothy McKenna, CP2M UMR 5128, France
- 4. Combining 13C-NMR triad sequence data with joint molecular weight and composition data to estimate parameters in a gas-phase polyethylene reactor model Jakob Straznicky, Queen's University, Canada
- 5. Modeling and parameter estimation for gas-phase polyethylene product properties using dynamic and steady-state data Lauren Gibson, Queen's University, Canada
- Turbidity spectroscopy as a potential tool to online monitor emulsion polymerization processes Usue Olatz Aspiazu, POLYMAT (Universidad del País Vasco/Euskal Herriko Unibertsitatea), Spain
- 7. Influence of pH on the kinetics of polymer hydrolysis: The case of polylactic acid Flavio Tollini, Politecnico di Milano, Italy
- 8. **Functionalized lactic acid macromonomers polycondensation** Flavio Tollini, Politecnico di Milano, Italy
- 9. **Chemical and optical mixing characterization of a dynamic inline mixer** Wladislaw Dolshanskiy, Universität Hamburg, Germany
- 10. **Reactive molding of elastomers in 3D-printed molds for robotic actuators** Alexey Stepanyuk, Technische und Molekulare Chemie, University of Hamburg, Germany
- 11. **Enzimatic polycondensation of 1,4-butanediol and diethyl succinate** Claudia Sayer, UFSC, Brazil
- 12. Encapsulation of aqueous-core nanocapsules in PLLA multicompartments microparticles Claudia Sayer, UFSC, Brazil
- 13. **Influence of reaction conditions on the solution polymerization of vinyl acetate** Kristina Zentel, TU Darmstadt, Germany
- 14. **Solubility of multiple gases in amorphous polypropylene** Kusuma Kulajanpeng, Université Claude Bernard Lyon 1, France
- 15. A study of the radical polymerization kinetics of 2-(Dimethylamino) ethyl methacrylate in aqueous solution in the presence of monomer ionization and hydrolysis Robin A. Hutchinson, Queen's University, Canada
- 16. **Computational approach for procedural generation of protein-DNA architectures** Thor van Heesch, University of Amsterdam, the Netherlands

- 17. Engineering polymers to study structure/property relationships in desalination membranes Sean Bannon, University of Virginia, USA
- Emulsion polymerization of very hydrophobic bio-based monomers: Challenges and limitations Aitor Barquero, UPV/EHU, Spain
- Disentangled UHMWPE Control of crystallization, chain entanglement and rheology via process conditions Roberta Lopes do Rosario, CP2M UMR 5128, France
- 20. The synthesis of isobornyl acrylate macromonomers for structured copolymer dispersants by high-temperature semi-batch radical polymerization Elizabeth Bygott, Queen's University, Canada

Engineering Conferences International

Engineering Conferences International (ECI) is a not-for-profit global engineering conferences program that has served the engineering/scientific community since 1962 as successor program to Engineering Foundation Conferences. ECI has received recognition as a 501(c)3 organization by the U.S. Internal Revenue Service and is incorporated in the State of New York as a not-for-profit corporation.

The program has been developed and is overseen by volunteers both on the international Board of Directors and international Conferences Committee. More than 1,900 conferences have taken place to date. The conferences program is administered by a professional staff and the conferences are designed to be self-supporting.

ECI Mission

To serve the engineering/scientific community with international, interdisciplinary, leading edge engineering research conferences

ECI Purposes

The advancement of engineering arts and sciences by providing a forum for the discussion of advances in the field of science and engineering for the good of mankind by identification and administration of international interdisciplinary conferences

To work with engineering, scientific and social science societies and the interested general public to jointly sponsor conferences and to take other actions that will foster complementary programming.

To initiate conferences that will have a significant impact on engineering education, research practice and/or development.

ECI Encouragement of New Conference Topics

The ECI Conferences Committee invites you to suggest topics and leaders for additional conferences and encourages you to submit a proposal for an ECI conference.

Ideally, proposals should be submitted from 18 to 24 months in advance of the conference although the staff can work on a shorter timeline.

The traditional format for an ECI conference is registration Sunday afternoon with technical sessions held each morning and evening through Thursday or Friday noon. Afternoons are used for informal gatherings, poster sessions, field trips, subgroup meetings and relaxation. This format has served well to build important professional networks in many areas.

ECI welcomes proposals for shorter conferences and for conferences which span weekends in order to reduce the number of working days participants are away from their offices.

ECI Works With You

ECI works with conference chairs in two complementary ways. First, an experienced member of the Conferences Committee acts as your technical liaison from the proposal stage through the conference itself. He or she is always available to consult with you on any conference issue.

Second, after your proposal has been approved by the Conferences Committee, the ECI staff will assume responsibility for the administration of the conference.

Your primary responsibilities will be recruiting the organizing committee, developing the technical program and securing third-party funding necessary to support the travel of key speakers.

The responsibilities of ECI's "full service" staff include -- but are not limited to -- the following:

- Recommend, negotiate, contract and make substantial deposits for housing, meals, meeting space, A/V equipment and tours.
- Maintain web sites for the conference and for submission of abstracts.
- Publicize via electronic and print media.
- Administer all finances including grants, contributions and purchase orders. (ECI makes grant funds available as soon as a grant is approved.) There is no need for chairs to set up a conference bank account or file tax returns for their conference.
- Process all applications and registrations.
- Produce bound program/abstracts book.
- Contract for the publication of print or electronic proceedings, if any.
- Provide on-site staff during the conference.

For more information, please contact the ECI Director at Barbara@engconfintl.org



Engineering Conferences International

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Calendar of ECI Conferences

Celebrating 60 years of international, interdisciplinary engineering conferences

| <u>2022</u> Oct 2-7 | 21AN | NANOMECHANICAL TESTING IN MATERIALS RESEARCH AND DEVELOPMENT VIII (Split, Croatia) S. Korte-Kerzel, RWTH Aachen University |
|----------------------------|--------------|---|
| Oct 9-13 | 22AA | INTEGRATED CONTINUOUS BIOMANUFACTURING V (Sitges, Spain) J. Walther, Sanofi; A. Azevedo, Instituto Superior Técnico; R. Deshpande, Amgen |
| Oct 30-Nov 3 | 20AE | ELECTROPHORETIC DEPOSITION VII: FUNDAMENTALS AND APPLICATIONS (Santa Fe, New Mexico) A.R. Boccaccini, Univ. of Erlangen-Nuremberg; B. Ferrari, Spanish Research Council; A.J. Pascall, Brookhaven National Laboratory; T. Uchikoshi, National Institute for Materials Science |
| Nov 13-18 | 21AS | CERAMIC MATRIX COMPOSITES II (Santa Fe, New Mexico) Y. Kagawa, Tokyo University of Technology; R. Darolia, GE Aviation (retired); R. Raj, University of Colorado; G. Singh, Kansas State University; D. Koch, University of Augsburg; G. Vignoles, University of Bordeaux; J. Binner, University of Birmingham |
| Dec 10-14 | 21AB | POLYMER REACTION ENGINEERING XI (Scottsdale, AZ) T. Mckenna, Universite Claude Bernard, France; C. Sayer, Federal University of Santa Catania, Brazil; J. Schork, Georgia Tech;USA; John Tsavalas, University of New Hampshire, USA; Jose Ramon Leiza, University of the Basque Country, Spain; Robin Hutchinson (Queen's University, Canada; Brian Greenhalgh, ExxonMobil Chemicals, USA; Markus Busch, TU Darmstadt, Germany; J Reimers, ExxonMobil Chemicals, USA |
| <u>2023</u> March 19-24 | 22AD | ELECTRIC FIELD ENHANCED PROCESSING OF ADVANCED MATERIALS III: COMPLEXITIES AND OPPORTUNITIES (Tomar, Portugal) R. Raj, University of Colorado at Boulder; Luis Perez-Maqueda, CICA, Spain |
| April 23-28 | 23AC | CELL CULTURE ENGINEERING XVIII (Cancun, Mexico) L. Palomares, IBT-UNAM; C. Goudar, Amgen; T. Wang, Roche |
| May 7-12 | 23AP | PYROLIQ II – 2023: Pyrolysis and Liquefaction of Biomass and Wastes (Hernstein, Austria) F. Berruti, ICFAR & Western University; A. Dufour, CNRS, ENSIC; M. Garcia-Perez, Washington State University; W. Prins, University of Ghent |
| May 14-17 | 23 AU | 2023 INTERNATIONAL CONFERENCE ON SEMICONDUCOR TECHNOLOGY FOR ULTRA LARGE SCALE INTEGRATED CIRCUITS AND THIN FILM TRANSISTORS (ULSIC VS TFT 8) (Hokkaido, Japan) Y. Kuo, Texas A&M University |
| May 28-June 2 | 21AG | ALKALI ACTIVATED MATERIALS AND GEOPOLYMERS: SUSTAINABLE CONSTRUCTION MATERIALS AND CERAMICS MADE UNDER AMBIENT CONDITIONS (Cetraro (Calabria), Italy) W.M. Kriven, University of Illinois at Urbana-Champaign; C. Leonelli, Universita' degli Studi di Modena e Reggio Emilia; J.L. Provis, University of Sheffield; A.R. Boccaccini, University of Erlangen-Nuremberg |
| June 18-23 | 23AI | INNOVATIVE MATERIALS FOR ADDITIVE MANUFACTURING II (IMAM II) (Tallin, Estonia D. Schmidt (Luxembourg Institute of Science and Technology (LIST); N. Gupta, New York University; E. Eastwood, DOE; B.G. Compton; University of Tennessee, Knoxville; G.M. Gladysz, Los Alamos National Laboratory |
| July 16-21 | 21AV | SIXTH INTERNATIONAL WORKSHOP ON STRESS-ASSISTED CORROSION DAMAGE (Washington, DC area) A.K. Vasudevan, Office of Naval Research (retired); R. Latanision, Exponent, Inc.; H. Holroyd, Luxfer (retired); F. Friedersdorf, Luna Innovations Inc. |

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| July 24-28 | 21AH | ASSOCIATION IN SOLUTION V (Azores, Portugal) I. Voets, Eindhoven University of Technology; J. Strakel, Wageningen University; J. Conrad, University of Houston |
|-----------------|-------|--|
| September 4-8 | 22AJ | TERATECH 2023: 10 th International Symposium on Terahertz-related Devices and Technologies (Aizu-Wakamatsu, |
| | | Japan) General Chair: Taiichi Otsuji, Tohoku University; LOC Chair: Maxim Ryzhii, University of Aizu, LOC Co-Chair: Junichiro Kono, Co-Chair of the LOC: Akira Satou, Tohoku University, Technical Program Chair: Junichiro Kono, Rice University; TPC Co- Chair: Alexey Belyanin, Texas A&M University |
| September 10-13 | 23AT | SINGLE USE TECHNOLOGIES VI (Boston, USA) M. Barbaroux, Sartorius; S. Kane, Takeda; S. Yoon, University of Massachusetts, Lowell |
| September 17-21 | 23-AH | INTERNATIONAL HYDROGEN CONFERENCE: UNDERSTANDING HYDROGEN-MATRIALS INTERACTIONS (Park City, Utah) M. Martin, NIST; J. Burns, University of Virginia |
| September 17-21 | 23AB | BIO-CHAR III (Tomar, Portugal) F. Berruti, Western University, Canada; D. Chiaramonti, Politecnico di Torino and RE-CORD, Italy; S. Fiore, Politecnico di Torino, Italy; M. Garcia-Perez, Washington State University, USA; O. Masek, University of Edinburgh, UK |
| October 1-6 | 23AE | ENZYME ENGINEERING XXVII (Singapore) Ang Ee Lui, A*Research, Singapore; Li Zhi, National University of Singapore; Yan Feng, Shanghai Jiao Tong University |
| Oct. 15-19 | 21AO | ADVANCES IN OPTICS FOR BIOTECHNOLOGY, MEDICINE AND SURGERY (Tomar, Portugal) M. Niedre, Northeastern University; F. Leblond, Polytecnique Montreal |
| <u>2024</u> | | |
| January 7-12 | 20AT | TRANSITION OF ENERGY SYSTEMS TOWARDS SUSTAINABILITY (Kolkata, India) S. De, S. Bandyopadhyay, IIT, Bombay |
| February 4-8 | 24AT | ADVANCING MANUFACTURE OF CELL AND GENE THERAPIES VIII (Coronado, CA) F. Masri, Cell & Gene Catapult; C. Yeager, Georgia Institute of Technology; G. Maheshwari, BMS; J. Moscariello, BMS |
| February TBA | 21AD | ADVANCED MEMBRANE TECHNOLOGY VIII: ENVIRONMENT, FOOD, HEALTH AND NEW FRONTIERS (Casablanca, Morocco) J. Hestekin, University of Arkansas; U. Beusche, W.L. Gore, Inc.; D. Bhattacharyya, University of Kentucky |
| April 4-7 | 20AP | DELIVERY OF NUCLEIC ACID THERAPEUTICS II: BIOLOGY, ENGINEERING AND DEVELOPMENT (Siracusa, Sicily) |
| | | L. Sepp-Lorenzino, Intellia Therapeutics; S. F. Dowdy, University of California San Diego School of Medicine; M. Stanton, Generational Bio |
| Spring | 24AI | ULTRA-HIGH TEMPERATURE CERAMICS: MATERIALS FOR EXTREME ENVIRONMENT APPLICATIONS V (Sicily,Italy) D. Sciti, Institute for Science and Technology of Ceramics, CNR; |
| April TBA | 24AK | MICROBIAL ENGINEERING III (TBA) E. Keshavarz-Moore, University College London; T. Sauer, Sanofi |
| April/May | 20AF | SYNTACTIC AND COMPOSITE FOAMS (Riga, Latvia) G.M. Gladysz and K.K. Chawla, University of Alabama at Birmingham; A. R. Boccaccini, University of Erlangen-Nuremberg; M. Fukushima, National Institute of Advanced Industrial Science and Technology |
| ТВА | 24AH | NANOTECHNOLOGY IN MEDICINE III: ENABLING NEXT GENERATION THERAPIES (TBA) K. Rege, Arizona State University; S. De Smedt, Ghent University S. Varghese, Duke University |
| May 19-24 | 24AA | VACCINE TECHNOLOGY IX (Los Cabos, Mexico) C. Lutsch, Sanofi Pasteur; L. Lua, University of Queensland; F. Godia, Universitat Autònoma de Barcelona; T. Tagmyer, Merck |
| ТВА | 24AM | BIOCHEMICAL AND MOLECULAR ENGINEERING XXIII (TBA) M. O'Malley, University of California at Santa Barbara; B. Pfleger, University of Wisconsin |
| Sept/Oct | 24AW | WATER (Europe) D. Hunkeler, Aqua+Tech; |
| Oct 6-11 | 24AN | NANOMECHANICAL TESTING IN MATERIALS RESEARCH AND DEVELOPMENT IX (Sicily, Italy) M. Sebastiani, Rome TRE University |
| Fall | 24AB | INTEGRATED CONTINUOUS BIOMANUFACTURING VI (USA) A. Azevedo, Instituto Superior Técnico; A. Noyes, Codiak Bio;; K. Brower, Sanofi |

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