Emulsion Polymers Consulting and Education, LLC presents

*Basics of Creating Latex Particles with Controlled Size and Chemistry**

NASA Website Photo

An On-line, Interactive Workshop August 23-26, 2021

Faculty

Donald C. Sundberg, PhD
Michael F. Cunningham, PhD

* Emulsion Polymers Consulting and Education (EPCEd) has a curriculum of 9 interactive workshops under the umbrella of the Science and Technology of Emulsion Polymers, or STEPn. This workshop is STEP1.

WORKSHOP OBJECTIVES: Despite having been practiced at commercial scales for more than a century, emulsion polymerization is increasingly the preferred reaction process used to create polymers of high molecular weight as aqueous based dispersions. The latex product is in the form of nanoparticles with controllable chemistry, and even extends to multicomponent particle systems with specific morphological structures. A thorough review of free radical polymerization reactions for homo- and comonomer systems establishes the basis for understanding the chemical kinetics that take place in both the water and polymer particle phases. Extension to the physical chemistry of colloidal systems allows us to establish the principles that control nanoparticle nucleation and subsequent growth.

INTENDED AUDIENCE: This workshop has been designed to introduce those relatively new to this field to the chemical and physical principles involved in creating latex particles with controlled polymer chemistry and nanoparticle size distributions. By developing a solid background in these subjects, participants will then be well positioned to work with the myriad of challenges involved in creating commercially viable latex based polymers.

STRUCTURE OF THE WORKSHOP: This on-line workshop will be presented in 4-hour segments over the four days in August. Daily starting times are planned to be at 9:30 AM (EDT). Sessions will be conducted in an ***interactive manner*** with participants engaged in problem solving and facilitated discussions.

WORKSHOP OUTLINE: See next page for a complete schedule of topics. Faculty profiles follow on page 4.

REGISTRATION INFORMATION

The registration fee includes the full book of workshop slides delivered to the registrant's home or business address. Presentations will be made on-line via Microsoft Teams. ***Early registration is recommended*** due to the workshop size limitation of 30 participants.

Registration Fee: ***$1200 USD***
Registration Form – **Go To Page 5**

Contact for further information:
info@epced.com

Basics of Creating Latex Particles with Controlled Size and Chemistry

Session 1

- Course introduction and overview
- Course objectives and expectations of participants
- Basic chemical mechanisms and modes of reaction for emulsion polymers
    1. Free radical polymerization reactions
    2. Polymer chain characteristics, radius of gyration, entanglements
    3. Chain structure – linear, branched, grafted, crosslinked
    4. Reaction rates in free radical polymerization
        - Homopolymerization – free radical and monomer concentrations, influence of temperature and viscosity
        - Copolymerization – reactivity ratios, cross-termination, copolymer composition control, chain transfer to polymer reactions
    5. Molecular weight control
        - Chain growth and stopping events, number average chain length
        - Molecular weight distributions, most probable distribution, dependence on monomer and radical concentrations, chain transfer agent
    6. Modes of reaction
        - Batch reactions – time dependencies, reaction rates
        - Semi-batch reactions – monomer feeding profiles, control of monomer concentrations, copolymer composition control, temperature variations, residual monomers

Session 2

- **Creating polymer particles in emulsion polymerization**
    1. Chemical and physical mechanisms involved in batch reactions
    2. Physical chemistry of surfactant micelles
    3. Initiation of radicals in water phase, z-mer concept, radical entry
    4. 3-time intervals of reaction, distinctive boundaries between intervals
    5. Homogeneous nucleation of particles (without micelles)
    6. Particle size control
        - *Ab initio*
        - Growth from seed
        - Control of particle size distribution
- **Details for rates of reaction during emulsion polymerization**
    1. Smith-Ewart approach – quantitative – difference equations
        - Cases for nbar = 1/2 --- instantaneous termination in latex particles
        - Cases for nbar < 1/2 --- radical exit
        - Cases for nbar > 1/2 --- diffusion controlled termination, pseudo bulk
    2. Batch reaction rates vs. time of reaction (conversion), Intervals I, II and III
    3. Semi-batch processing alternatives
        - Why use semi-batch?
        - Effect on [M] and on polymer viscosity in particles
            a) How far can radicals penetrate into particles?
            b) How do polymer particles grow? Accretion? Monomer swelling?
            c) Effect of polymer T_g and [M] on reaction rates; diffusion controlled termination, chain transfer to polymer in acrylates
            d) Residual monomer

4. Initiator systems
    - Thermal dissociation
        a) Water phase initiation, oil phase initiation
        b) Initiator end groups, especially for water phase initiation
        c) Dead end polymerization, feeding initiator during process
    - Redox systems
        a) Commonly used oxidant/reductant pairs
        b) Reactivity of oxygen vs. carbon centered radicals
        c) Initiator efficiencies (oil phase, water phase)
    - Methods of addition – distinguish between addition during polymerization process and during the finishing operation (to remove residual monomer)

<u>Session 3</u>

- **Details for latex particle size control**
    1. *Ab initio* processes in batch process
        - Micellar mechanism
        - CMC values; temperature and ionic strength effects
        - Interval I in Harkins mechanism of particle formation
            a) Time and conversion duration of this interval
            b) Possible size difference between youngest and oldest particles
        - Intervals II and III in Harkins mechanism
            a) Particle growth during interval II; monomer concentration in particles
            b) Interval III (no growth); finishing the polymerization
        - Colloidal stability during Intervals I and II
            a) Controlling surfactant coverage
            b) Consequences of too much surfactant (secondary nucleation)
            c) Consequences of too little surfactant during growth interval – coagulation
    2. *Seeded* latex particle growth
        - Size of seed vs. final, desired size, stage ratio
        - Residual surfactant and initiator in seed latex – possible need for extra
        - Monomer feed alternatives
            a) Batch process; [M] in particles at start of seeded reaction
            b) Semi-batch; *starved* and flooded conditions
            c) Power feeds for some copolymer systems
            d) Reaction rates during semi-batch operations
- **Details for molecular weight control**
    1. Kinetic chain length, <X_N>; special considerations for emulsion polymerization
        - Radical entry rate
        - Chain termination in particles; long-short termination
        - Chain transfer to monomer effects (only in batch reactions)
        - Chain transfer to external agents
            a) Solubility in water issues
            b) Transport to latex particles
            c) Chain transfer constants

<u>Session 4</u>

- **Details for molecular weight control, continued**
    2. Molecular weight distributions (MWD)
        - Linear chains; changing conditions of [M] and radical entry rates
        - Branching reactions; chain transfer to polymer, addition of divinyl monomers
        - Crosslinking reactions; natural/inherent as in acrylates and dienes; with added divinyl monomers
    - **Details for copolymer composition control**
    1. Batch reactions
    2. Semi-batch reactions
- **Introduction to colloidal stability**
    1. Electrostatic stability mechanism; temperature and ionic strength issues
    2. Steric stability; entropy considerations, non-ionic stabilizers
- **Review of important lessons learned and conclusion of workshop**

Faculty Profiles

Professor Donald C. Sundberg has been working in the field of emulsion polymers for 53 years. He received a bachelor's degree in chemical engineering from Worcester Polytechnic Institute (Massachusetts) and his Ph.D. from the University of Delaware. He worked on latex based impact modifiers for ABS resins with the Monsanto Company, scaling processes to the 10,000 gallon reactor size. He has extensive research experience in emulsion polymerization and is widely recognized for his work on structured latex particles. This has resulted in over 100 peer reviewed publications and many conference papers. In addition he has conducted many workshops, most notably the one on latex particle morphology control. He spent a sabbatical year at the Institute for Surface Chemistry in Stockholm and was Chair of the 1997 Gordon Research Conference on Polymer Colloids. He is the 2016 Mattiello Memorial Lecture awardee from the American Coatings Association. His research interests are in polymerization kinetics in solution, bulk and emulsion systems, interfacial science and polymer morphology control, diffusion in polymers, and coatings. He is an Emeritus Professor of Materials Science at the University of New Hampshire and is the founder of Emulsion Polymers Consulting and Education, LLC.

Professor Michael F. Cunningham has an extensive background in dispersed phase polymerizations, including suspension, emulsion, miniemulsion and dispersion polymerization. He received a bachelor's degree in Engineering Chemistry from Queen's University (Kingston, Ontario, Canada) and his Ph.D. from the University of Waterloo. He spent six years working on dispersed phase polymerizations in the Xerox Corporate Research Group, acquiring experience in process scaleup and technology transfer to manufacturing. He has an active research program in polymer colloids and emulsion polymerization, particularly in the area of living radical polymerization and stimuli-responsive particles, publishing over 200 peer reviewed publications, and holding 26 U.S. patents. He is secretariat of the International Polymer Colloids Group, and previously held the Ontario Research Chair in Green Chemistry and Engineering. He has consulted with a number of companies in the area of emulsion and suspension polymerization, and lectured for over 10 years at industrial short courses on emulsion polymerization in the USA and Switzerland. He is a Partner with Professor Sundberg in the international consulting firm Emulsion Polymers Consulting and Education, LLC.

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On-line workshop
August 23-26, 2021
Registration Form

Name____
Address____
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City/State____
Postal Code____
Country____
Position or Title_____________________________________
Organization____
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Participant Category
☐ Standard price for industrial participant: $1200 (USD)
☐ Discounted price for ***additional*** participant(s) from the same company: $1100 (USD)
☐ Academic participant: $1000 (USD)

There is a non-refundable fee of $50 (USD). Cancellation of registration can be made up until July 23, 2021 with a full refund less the $50 processing fee.

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