Second Edition









# Crystallization of Organic Compounds

An Industrial Perspective

Hsien-Hsin Tung Edward L. Paul Michael Midler James A. McCauley

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# <u>Crystallization Of Organic Compounds An Industrial</u> <u>Perspective</u>

Hsien-Hsin Tung, Edward L.
Paul, Michael Midler, James A.
McCauley

#### **Crystallization Of Organic Compounds An Industrial Perspective:**

Crystallization of Organic Compounds Hsien-Hsin Tung, Edward L. Paul, Michael Midler, James A. McCauley, 2023-07-05 Crystallization of Organic Compounds Practical resource covering applications of crystallization principles with methodologies case studies and numerous industrial examples for emphasis Based on the authors hands on experiences as process engineers through the use of case studies and examples of crystallization processes ranging from laboratory development through manufacturing scale up Crystallization of Organic Compounds guides readers through the practical applications of crystallization and emphasizes strategies that have proven to be successful enabling readers to avoid common pitfalls that can render standard procedures unsuccessful Most chapters feature multiple examples that guide readers step by step through the crystallization of active pharmaceutical ingredients APIs including an analysis of the major methods of carrying out crystallization operations their strengths and potential issues as well as numerous examples of crystallization processes from development through manufacturing scale Advancements in the field of crystallization have been integrated throughout the book in the newly revised Second Edition to ensure the content adequately reflects current state of the art industrial know hows and practice The new edition also adds chapters addressing downstream operations after the crystallization including filtration washing and drying together with industrial use cases Crystallization of Organic Compounds includes detailed information on Solubility and solid behavior covering phase rule polymorph salt co crystal chiral resolution and in silico solubility prediction and kinetics covering seed supersaturation nucleation crystal growth and model based experimental design Critical issues in the crystallization practice covering oiling out seeding wet milling agglomeration aggregation mixing scale up and quality by design principles Cooling anti solvent evaporation and reactive crystallization process design covering batch and continuous operations with industrial examples Special applications covering crystallization with ultrasound reaction selectivity enhancement and computation fluid dynamics and solid dispersion With highly practical coverage of the subject Crystallization of Organic Compounds is an essential resource for engineers and chemists involved with the development scaling or operation of crystallization process in the pharmaceutical and fine chemical industries particularly those with degrees in chemical engineering and chemistry Crystallization of Organic Compounds Hsien-Hsin Tung, Edward L. Paul, Michael Midler, James A. McCauley, 2009-06-09 Filled with industrial examples emphasizing the practical applications of crystallization methodologies Based on the authors hands on experiences as process engineers at Merck Crystallization of Organic Compounds guides readers through the practical aspects of crystallization It uses plenty of case studies and examples of crystallization processes ranging from development through manufacturing scale up The book not only emphasizes strategies that have been proven successful it also helps readers avoid common pitfalls that can render standard procedures unsuccessful The goal of this text is twofold Build a deeper understanding of the fundamental properties of crystallization as well as the impact of these properties on crystallization

process development Improve readers problem solving abilities by using actual industrial examples with real process constraints Crystallization of Organic Compounds begins with detailed discussions of fundamental thermodynamic properties nucleation and crystal growth kinetics process dynamics and scale up considerations Next it investigates modes of operation including cooling evaporation anti solvent and reactive crystallization. The authors conclude with special applications such as ultrasound in crystallization and computational fluid dynamics in crystallization Most chapters feature multiple examples that guide readers step by step through the crystallization of active pharmaceutical ingredients APIs With its focus on industrial applications this book is recommended for chemical engineers and chemists who are involved with the development scale up or operation of crystallization processes in the pharmaceutical and fine chemical industries **Crystallization of Organic Compounds** Hsien-Hsin Tung, Edward L. Paul, Michael Midler, James A. McCauley, 2009-06-17 Filled with industrial examples emphasizing the practical applications of crystallization methodologies Based on the authors hands on experiences as process engineers at Merck Crystallization of Organic Compounds guides readers through the practical aspects of crystallization It uses plenty of case studies and examples of crystallization processes ranging from development through manufacturing scale up The book not only emphasizes strategies that have been proven successful it also helps readers avoid common pitfalls that can render standard procedures unsuccessful The goal of this text is twofold Build a deeper understanding of the fundamental properties of crystallization as well as the impact of these properties on crystallization process development Improve readers problem solving abilities by using actual industrial examples with real process constraints Crystallization of Organic Compounds begins with detailed discussions of fundamental thermodynamic properties nucleation and crystal growth kinetics process dynamics and scale up considerations. Next it investigates modes of operation including cooling evaporation anti solvent and reactive crystallization. The authors conclude with special applications such as ultrasound in crystallization and computational fluid dynamics in crystallization Most chapters feature multiple examples that quide readers step by step through the crystallization of active pharmaceutical ingredients APIs With its focus on industrial applications this book is recommended for chemical engineers and chemists who are involved with the development scale up or operation of crystallization processes in the pharmaceutical and fine chemical industries *Industrial Crystallization* Gerard Capellades, Fredrik L. Nordstrom, 2025-06-12 The goal of this primer is to introduce crystallization to newcomers in the field with three primary readers in mind 1 new graduate students starting a crystallization project 2 scientists in industry who may be familiar with general chemistry and or crystallography and want to get an introduction to the topics behind crystallizer design and 3 students taking a crystallization elective course or a crystallization module in a broader separations course Contrary to a textbook or review article this is a digital primer where the authors prioritize simplicity over completeness and breadth over depth Each chapter in the primer contains selected references such as Read These Next for those who wish to dive deeper into a specific topic Crystallization can be found in multiple areas within materials design and

separations The product of a crystallization step may be a single crystal or a powder It may be composed of small organic molecules inorganic salts biological molecules or single elements Similarly it may have been crystallized from its molten state or pre dissolved in an appropriate solvent and then crystallized via e g cooling antisolvent addition a chemical reaction or solvent evaporation Each of these combinations may be their field of research requiring very different approaches and considerations that warrant their primers This primer focuses on solvent mediated crystallization as a separation process often called solution crystallization with solid liquid suspensions being the main product **Industrial Crystallization Process Monitoring and Control** Angelo Chianese, Herman J. Kramer, 2012-04-16 Crystallization is an important technique for separation and purification of substances as well as for product design in chemical pharmaceutical and biotechnological process industries This ready reference and handbook draws on research work and industrial practice of a large group of experts in the various areas of industrial crystallization processes capturing the essence of current trends the markets design tools and technologies in this key field Along the way it outlines trouble free production provides laboratory controls analyses case studies and discusses new challenges First the instrumentation and techniques used to measure the crystal size distribution the nucleation and solubility points and the chemical composition of the solid and liquid phase are outlined Then the main techniques adopted to control industrial crystallizers starting from fundamental approaches to the most advanced ones including the multivariable predictive control are described An overview of the main crystallizer types is given with details of the main control schemes adopted in industry as well as the more suitable sensors and actuators

Crystallization Marcello Andreeta, 2012-09-19 Crystallization is one of the most ancient and interdisciplinary topics of research known to mankind Crystals can be organic or inorganic and may be produced from melts liquid solutions vapors or even in solid state Notwithstanding its inherently high complexity the crystallization process is part of our everyday lives from ice making in our homes to the most state of the art chemical and electronic industry In this book our purpose was to present new insights to the reader as well as crucial and very useful information for researchers working in this field while simultaneously creating a comprehensive text about crystallization processes which may serve as a starting point for people with different backgrounds Reactive Crystallization of Terephthalic Acid towards Recycling of Poly(ethylene terephthalate) Clemens Müller, 2025-06-11 Die vorliegende Arbeit behandelt Untersuchungen der reaktiven Kristallisation von Terephthals ure TA im Rahmen des Back tot Monomer Recyclings welches eine M glichkeit zur berwindung der derzeitigen Limitierungen des thermomechanischen Polyethylenterephthalat PET Recyclings darstellt Ein Ansatz ist dabei die alkalische Hydrolyse bei welcher PET mit Natriumhydroxid selektiv in die Monomere Ethylenglykol und Dinatriumterephthalat depolymerisiert wird Anschlie end wird die TA durch S urezugabe aus ihrem Dinatriumsalz gef llt und so zur ckgewonnen Zur Optimierung der F llung als Gewinnungsschritt wurden verschiedene Betriebsparameter hinsichtlich ihres Effekts auf Kristallgr e Filtrierbarkeit und Reinheit der TA analysiert Dazu wurde zun chst ein Parameterscreening mit

Modelll sung im Batchbetrieb durchgef hrt Hierbei f hrten insbesondere erh hte Temperaturen und Essigs ureeinsatz zu gr eren Kristallen und verbesserter Filtrierbarkeit Trotz ihrer geringeren Protonierungskapazit t wurde auch mit Essigs ure eine signifikante Ausbeute an TA erreicht Anschlie end wurden die Untersuchungen auf depolymerisiertes PET verschiedener Abfallfraktionen und das Aufreinigungspotential der F llung ausgeweitet Neben einer Verringerung der Verf rbung bei h herer Temperatur wurde auch der Isophthals uregehalt in TA Kristallen reduziert was sich insbesondere bei Verwendung von Essigs ure zeigte Dies ist insbesondere relevant da Isophthals ure einen entscheidenden Einfluss auf die Polymereigenschaften hat Im letzten Teil der Arbeit wurden die Untersuchungen in einen kontinuierlichen R hrkessel berf hrt W hrend der F llung mit Schwefels ure konnte so ein Wachstum der TA Kristalle einhergehend mit einer verbesserten Filtrierbarkeit erreicht werden Dar ber hinaus induzierte eine Erh hung des pH Werts eine signifikante Reduktion des Isophthals uregehalts Schlie lich wurde ein Verfahrenskonzept f r einen optimierten F llungsschritt f r TA hinsichtlich Reinheit und R ckgewinnung abgeleitet unter Beachtung der Notwendigkeit eines nachfolgenden Umkristallisationsschritts

Conceptual Design of Crystallization Processes Christianto Wibowo, Ka Ming Ng, 2020-11-23 The book presents in a unified manner various crystallization design methods It discusses in detail the geometric framework for representing complex phase behavior involving multiple solutes enantiomers hydrates compounds polymorphs and solid solutions through visualization of high dimensional phase diagrams It also describes how the impact of transport processes is accounted for using kinetically controlled process paths **Separation Process Engineering Phillip C. Wankat, 2022-10-24 The** Definitive Learner Friendly Guide to Chemical Engineering Separations Extensively Updated Including a New Chapter on Melt Crystallization Efficient separation processes are crucial to addressing many societal problems from developing new medicines to improving energy efficiency and reducing emissions Separation Process Engineering Fifth Edition is the most comprehensive accessible guide to modern separation processes and the fundamentals of mass transfer In this completely updated edition Phillip C Wankat teaches each key concept through detailed realistic examples using actual data with up to date simulation practice spreadsheet based exercises and references Wankat thoroughly covers each separation process including flash column and batch distillation exact calculations and shortcut methods for multicomponent distillation staged and packed column design absorption stripping and more His extensive discussions of mass transfer and diffusion enable faculty to teach separations and mass transfer in a single course And detailed material on liquid liquid extraction adsorption chromatography and ion exchange prepares students for advanced work New and updated content includes melt crystallization steam distillation residue curve analysis batch washing the Shanks system for percolation leaching eutectic systems forward osmosis microfiltration and hybrid separations A full chapter discusses economics and energy conservation including updated equipment costs Over 300 new and updated homework problems are presented all extensively tested in undergraduate courses at Purdue University New chapter on melt crystallization solid liquid phase equilibrium suspension

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