



DECHEMA

Gesellschaft für Chemische Technik
und Biotechnologie e.V.

PROGRAMME

30 August – 2 September 2021 · Online Event

ISIC 21

21st International Symposium on Industrial Crystallization

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Monday, 30 August 2021

	Tutorial A	Tutorial B	
9:00-12:30	Industrial Crystallization Fundamentals J. ter Horst/F	Industrial Aspects of Crystallization M. Stepanski/CH	
	Virtual Room 1		
	Welcome and Opening		
13:00	WELCOME & OPENING REMARKS		
Chair	H. Lorenz/D		
13:10	PLENARY OPENING LECTURE J.M. Garcia Ruiz/E		
13:50	KEYNOTE LECTURE J. ter Horst/F		
14:15	Discussion with speakers		
14:30	Coffee Break		
	Virtual Room 1	Virtual Room 2	Virtual Room 3
	Kinetics I	Separation of Enantiomers I	Integrated Processes I
Chair	A. Myerson/USA	G. Coquerel/F	E. Verdurand/CH
14:45	S. Kulkarni/USA	F. Breviglieri/CH	J. von Langermann/D
15:05	L. Bosetti/CH	C. Xiouras/B	Z. Nagy/UK & USA
15:25	S. Schiele/D	M. Charpentier/UK	M. Spicher/D
15:45	R. Miller/UK	S. Bhandari/D	Discussion with speakers
16:05	Discussion with speakers	Discussion with speakers	
16:25 17:30	Opening Poster Discussion / Session I		
18:00	Social Get-together: Quiz		

Time: CEST

4 POSTER PRIZES

sponsored by



will be awarded in the closing session.

Tuesday, 31 August 2021

	Virtual Room 1	Virtual Room 2	Virtual Room 3
	Process Monitoring	Separation of Enantiomers II	Industrial Applications I
<i>Chair</i>	<i>M. Louhi-Kultanen/FIN</i>	<i>M. Mazzotti/CH</i>	<i>P. Carvin/F</i>
8:30	J. Lins/D	B. Bodák/CH	A. Zwijnenburg/NL
8:50	T. Kathyola/UK	K. Funakoshi/J	J. Gebauer/D
9:10	D. Wirz/D	J. Sun/CN	A. Collas/B
9:30	A. Jaeggi/CH	F. Cascella/D	I. Østergaard/DK
9:50	Discussion with speakers	Discussion with speakers	Discussion with speakers
10:10	Coffee Break		
10:30	Poster Session II		
12:00	Lunch Break		
	Virtual Room 1		
	Plenary and Keynote Lectures		
<i>Chair</i>	<i>R. Geertman/B</i>		
12:45	PLENARY LECTURE C. Melches/D		
<i>Chair</i>	<i>A. Zwijnenburg/NL</i>		
13:25	KEYNOTE LECTURE E. Rigaut/CH		
13:50	KEYNOTE LECTURE A. Chow/SGP		
14:15	Discussion with speakers		
14:30	Coffee Break		
	Virtual Room 1	Virtual Room 2	Virtual Room 3
	Kinetics II	Continuous Crystallization	Industrial Applications II
<i>Chair</i>	<i>P. Daudey/NL</i>	<i>Z. Nagy/UK & USA</i>	<i>M. Lee/UK</i>
14:50	G. Kaysan/D	N. Rey/CH	C. Burcham/USA
15:10	A. Cashmore/UK	K. Tacsí/H	H. Yao/USA & B. Williams/UK
15:30	D. Guse/D	J. Gänsch/D	T. Rosenbaum/USA
15:50	Discussion with speakers	Discussion with speakers	Discussion with speakers
16:05	Short Break		
	Virtual Room 1		
	Plenary Lecture		
<i>Chair</i>	<i>A. Seidel-Morgenstern/D</i>		
16:15	PLENARY LECTURE R. Braatz/USA		
17:00	End of second day		
17:15	WP Meeting in the evening (invited participants)		

Wednesday, 1 September 2021

	Virtual Room 1	Virtual Room 2	Virtual Room 3
	Modeling	Reactive Crystallization	Contributions to Sustainability
<i>Chair</i>	<i>D. Marchisio/I</i>	<i>B. Biscans/F</i>	<i>A. Lewis/ZA</i>
8:30	J. Unno/J	J. Gómez-Morales/E	F. Vassallo/I
8:50	V. Tenberg/D	H. Takiyama/J	L. Motsepe/ZA
9:10	C. Ma/UK	C. Ruiz Vasquez/F	M. Rodriguez Pascual/NL
9:30	M. Ukrainczyk/IRL	L. Metzger/D	R. Halfwerk/NL
9:50	Discussion with speakers	Discussion with speakers	Discussion with speakers
10:10	Coffee Break		
10:30	Poster Session III		
12:00	Lunch Break		
	Plenary and Keynote Lectures		
<i>Chair</i>	<i>C. Melches/D</i>		
12:45	PLENARY LECTURE B. Biscans/F		
<i>Chair</i>	<i>M. Stepanski/CH</i>		
13:25	KEYNOTE LECTURE D. Marchisio/I		
13:50	KEYNOTE LECTURE R. Rousseau/USA		
14:15	Discussion with speakers		
14:30	Coffee Break		
	Virtual Room 1	Virtual Room 2	Virtual Room 3
	Crystalline Phase Behaviour	Battery Materials	Integrated Processes II
<i>Chair</i>	<i>J. Gomez Morales/E</i>	<i>M. Rauls/D</i>	<i>B. Glennon/IRL</i>
14:50	Y. Liu/CN	M. Para/I	C. Steenweg/D
15:10	R. Mani/FIN	R. Berk/D	W. Wu/USA
15:30	F. Marques Penha/S	M. Le Page Mostefa/F	N. Mitchell/UK
15:50	Discussion with speakers	Discussion with speakers	Discussion with speakers
16:05	Short Break		
	Plenary Lecture		
<i>Chair</i>	<i>M. Rauls/D</i>		
16:15	PLENARY LECTURE D. Green/USA		
17:00	End of third day		

Thursday, 2 September 2021

	Virtual Room 1	Virtual Room 2	Virtual Room 3
	Microfluidic Techniques	Lectures to Honor Gerda v. Rosmalen & Special Techniques	Special Techniques
<i>Chair</i>	<i>K. Wohlgemuth/D</i>	<i>J. ter Horst/F & H. Wei/CN</i>	<i>A. Chow/SGP</i>
8:30	F. Ibis/NL	A. Lewis/ZA	S. Shikha/SGP
8:50	G. Peybernes/F	B. Eral/NL	W. Tian/UK
9:10	R. Cedeno/F	K. Tanaka/J	J. Wang/CN
9:30	A. Nelson/SGP	N. Ramos/D	S. Kwon/HK
9:50	Discussion with speakers	Discussion with speakers	Discussion with speakers
10:10	Coffee Break		
10:30	Poster Session IV		
11:30	Lunch Break		
	Plenary and Keynote Lectures		
<i>Chair</i>	<i>H. Lorenz/D & M. Mazzotti/CH</i>		
12:15	PLENARY LECTURE H. Cölfen/D		
12:55	KEYNOTE LECTURE A. Pallipurath/UK		
13:20	EFCE PRIZE AWARD LECTURE 2020 / 2021 A.K. Rajagopalan/CH		
13:45	Discussion with speakers		
14:00	Closing & Announcement of ISIC 22		
14:15	End of lecture programme		
14:30	Tutorial C Modeling, Monitoring & Control Z. Nagy/UK & USA		
17:30	End of the conference		

Monday, 30 August 2021

09:00 – 12:30

TUTORIAL A

Industrial Crystallization Fundamentals

J. ter Horst¹, E. Vlieg²; A. Flood³; ¹ Université de Rouen Normandie, Mont-Saint-Aignan/F; ² University of Nijmegen/NL; ³ Vidyasirimedhi Institute of Science and Technology (VISTEC), Wangchan, Rayong/TH

09:00 – 12:30

TUTORIAL B

Industrial Aspects of Crystallization

M. Stepanski¹; E. Verdurand²; C. Pudack³; E. Temmel¹; ¹ Sulzer Chemtech Ltd., Winterthur/CH; ² DSM Nutritional Products AG, Sisseln/CH; ³ KBR Plinke GmbH/D

Monday, 30 August 2021

Welcome and Opening

Virtual Room 1

13:00 **WELCOME & OPENING REMARKS**

Chair: H. Lorenz, Max Planck Institute for Dynamics of Complex Technical Systems & Otto von Guericke University, Magdeburg/D

13:10

PLENARY OPENING LECTURE**Wonderful crystal patterns in nature**

J.M. Garcia Ruiz¹; ¹ CSIC-University of Granada/E

13:50

KEYNOTE LECTURE**An Industrial Toolbox for Resolution & Deracemization of Chiral Compounds through Crystallization**

J. ter Horst¹; ¹ Université de Rouen Normandie, Mont-Saint-Aignan/F

14:15

Discussion with speakers

14:30

Coffee Break

Kinetics I

Virtual Room 1

Chair: A. Myerson, Massachusetts Institute of Technology, Cambridge/USA

14:45

A combined modeling and experimental approach to study the nucleation kinetics

S. Kulkarni¹; G. Wood¹; E. Santiso²; C. Liu²; F. Cao³; ¹ Pfizer Inc. Worldwide Research and Development, Groton/USA; ² North Carolina State University, Raleigh, North Carolina/USA; ³ Pfizer Inc. Worldwide Research and Development, La Jolla/USA

15:05

Surface secondary nucleation: the role of thermodynamics

L. Bosetti¹; B. Ahn¹; M. Mazzotti¹; ¹ ETH Zurich/CH

15:25

3D imaging yields a physical explanation for growth rate dispersion and size dependent growth

S. Schiele¹; R. Hupfer¹; H. Briesen¹; ¹ TU München, Freising/D

15:45

Modelling diffusive mixing in antisolvent crystallisation

R. Miller¹; J. Sefcik¹; L. Lue²; ¹ University of Strathclyde/ CMAC, Glasgow/UK; ² University of Strathclyde, Glasgow/UK

16:05

Discussion with speakers

16:25

Opening Poster Discussions / Poster Session I

17:30

18:00

Social Get-together: Quiz

Monday, 30 August 2021

09:00 – 12:30

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Industrial Crystallization Fundamentals

J. ter Horst¹, E. Vlieg²; A. Flood³; ¹ Université de Rouen Normandie, Mont-Saint-Aignan/F; ² University of Nijmegen/NL; ³ Vidyasirimedhi Institute of Science and Technology (VISTEC), Wangchan, Rayong/TH

09:00 – 12:30

TUTORIAL B

Industrial Aspects of Crystallization

M. Stepanski¹; E. Verdurand²; C. Pudack³; E. Temmel¹; ¹ Sulzer Chemtech Ltd., Winterthur/CH; ² DSM Nutritional Products AG, Sisseln/CH; ³ KBR Plinke GmbH/D

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14:15

Discussion with speakers

14:30

Coffee Break

Separation of Enantiomers I

Virtual Room 2

Chair: G. Coquerel, Université de Rouen/F

14:45

Improving the understanding of deracemisation via temperature cycles for enhanced process design and implementation

F. Breveglieri¹; B. Bodák¹; M. Mazzotti¹; ¹ ETH Zurich/CH

15:05

Development of continuous crystallization-enhanced deracemization processes with PAT monitoring

C. Xiouras¹; F. Cameli²; G. Belletti³; R. Venkatramanan⁴; H. Meekes³; E. Vlieg³; G. Stefanidis²; J. ter Horst⁴; ¹ Janssen Research & Development, Beerse/B; ² University of Leuven/B; ³ Radboud University, Nijmegen/NL; ⁴ University of Strathclyde, Glasgow/UK

15:25

Co-crystal screening: methods to optimize success rate

M. Charpentier¹; J. Devogelaer²; H. Meekes²; R. de Gelder²; E. Vlieg²; K. Johnston¹; J. ter Horst¹; ¹ University of Strathclyde, Glasgow/UK; ² Radboud University, Nijmegen/NL

15:45

A Shortcut Model to Evaluate Continuous Preferential Crystallization for Conglomerates Forming Systems

S. Bhandari¹; H. Lorenz²; A. Seidel-Morgenstern²; ¹ Otto von Guericke University Magdeburg/D; ² Max Planck Institut für Dynamik komplexer technischer Systeme / Otto-von-Guericke University Magdeburg/D

16:05

Discussion with speakers

16:25

Opening Poster Discussions / Poster Session I

17:30

18:00

Social Get-together: Quiz

Monday, 30 August 2021

09:00 – 12:30

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Industrial Crystallization Fundamentals

J. ter Horst¹, E. Vlieg²; A. Flood³; ¹ Université de Rouen Normandie, Mont-Saint-Aignan/F; ² University of Nijmegen/NL; ³ Vidyasirimedhi Institute of Science and Technology (VISTEC), Wangchan, Rayong/TH

09:00 – 12:30

TUTORIAL B

Industrial Aspects of Crystallization

M. Stepanski¹; E. Verdurand²; C. Pudack³; E. Temmel¹; ¹ Sulzer Chemtech Ltd., Winterthur/CH; ² DSM Nutritional Products AG, Sisseln/CH; ³ KBR Plinke GmbH/D

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J. ter Horst¹; ¹ Université de Rouen Normandie, Mont-Saint-Aignan/F

14:15

Discussion with speakers

14:30

Coffee Break

Integrated Processes I

Virtual Room 3

Chair: E. Verdurand, DSM Nutrition Products, Sisseln/CH

14:45

Integrated application and scale-up of a selective crystallization in an enzyme-catalysed synthesis process

J. Neuburger¹; D. Hülsewede¹; F. Belov¹; P. Süß²; U. Menyes²; J. von Langermann¹; ¹ University of Rostock/D; ² Enzymicals AG, Greifswald/D

15:05

A model-based framework for design and control of integrated crystallization, filtration and drying of active pharmaceutical ingredients

F. Destro¹; M. Barolo¹; Z. Nagy²; ¹ University of Padova/I; ² Purdue University, West Lafayette/USA

15:25

Upscaling the production of a novel, high potential phosphate binding nanomaterial

M. Spicher¹; S. Schwaminger¹; D. von der Haar-Leist²; S. Berensmeier¹; ¹ Technical University of Munich, Garching/D; ² Fraunhofer IVV, Freising/D

15:45

Discussion with speakers

16:00

End of session

16:25

Opening Poster Discussions / Poster Session I

17:30

18:00

Social Get-together: Quiz

Tuesday, 31 August 2021

Process Monitoring		Virtual Room 1
<i>Chair: M. Louhi-Kultanen, Aalto University, Espoo/FIN</i>		
08:30	Imaging techniques to understand and characterize agglomeration during batch cooling crystallization J. Lins ¹ ; U. Ebeling ¹ ; H. Ramezani ¹ ; K. Wohlgenuth ¹ ; ¹ TU Dortmund University, Dortmund/D	
08:50	Probing the Structural Evolution of a Molecular Solute in Solution with Advanced X-ray Analytical Techniques: A Study of Imidazole Crystallization L. Al-Madhagi ¹ ; B. Evans ¹ ; T. Kathyola ¹ ; E. Willneff ¹ ; S. Schroeder ¹ ; ¹ University of Leeds/UK	
09:10	Image-based inline measurement of crystal size distributions D. Wirz ¹ ; A. Seidel-Morgenstern ² ; M. Hofmann ¹ ; E. Temmel ³ ; H. Lorenz ⁴ ; H. Bart ¹ ; ¹ TU Kaiserslautern/D; ² Max Planck Institute for Dynamics of Complex Technical Systems & Otto von Guericke University, Magdeburg/D; ³ Sulzer Chemtech Ltd, Allschwil/CH; ⁴ Max Planck Institute for Dynamics Complex Technical Systems, Magdeburg/D	
09:30	Multidimensional Characterization of Platelets in Particulate Suspensions via Machine Learning A. Jaeggi ¹ ; A. Rajagopalan ¹ ; M. Morari ² ; M. Mazzotti ¹ ; ¹ ETH Zurich/CH; ² University of Pennsylvania, Philadelphia/USA	
09:50	Discussion with speakers	
10:10	Coffee Break	
10:30	Poster Session II	
12:00	Lunch Break	
Plenary and Keynote Lectures		Virtual Room 1
<i>Chair: R. Geertman, Janssen R&D BE, Beerse/B</i>		
12:45	PLENARY LECTURE Developments in large scale industrial crystallization R. Buchfink ¹ ; C. Melches ¹ ; H. Plate ¹ ; ¹ GEA Messo GmbH, Duisburg/D	
<i>Chair: A. Zwijnenburg, Nouryon Industrial Chemicals - Salt, Deventer/NL</i>		
13:25	KEYNOTE LECTURE An empirical modelling approach of layer crystallization supercharging strategies E. Rigaut ¹ ; E. Temmel ² ; M. Stepanski ¹ ; ¹ Sulzer Chemtech, Winterthur/CH; ² Sulzer Chemtech, Allschwil/CH	
13:50	KEYNOTE LECTURE Pharmaceutical cocrystals: from screening to process development and pre-formulation A. Chow ¹ ; ¹ Agency for Science, Technology & Research (A*STAR), Singapore/SGP	
14:15	Discussion with speakers	
14:30	Coffee Break	
Kinetics II		Virtual Room 1
<i>Chair: P. Daudey, TU Delft/NL</i>		
14:50	Possibilities and limitations of secondary contact nucleation of subcooled melt emulsions: A microfluidic approach G. Kaysan ¹ ; M. Kind ¹ ; ¹ Karlsruhe Institute of Technology (KIT), Karlsruhe/D	
15:10	Secondary Nucleation and Crystal Growth in the Metastable Zone A. Cashmore ¹ ; M. Haw ² ; M. Lee ³ ; J. Sefcik ¹ ; ¹ University of Strathclyde, CMAC Future Manufacturing Research Hub, Glasgow/UK; ² University of Strathclyde, Glasgow/UK; ³ GlaxoSmithKline, Stevenage/UK	
15:30	Experimental determination of solids formation times in the coprecipitation of Cu/Zn based catalyst precursors and their significance for catalyst preparation D. Guse ¹ ; S. Polierer ¹ ; S. Wild ¹ ; K. Herrera Delgado ¹ ; S. Pitter ¹ ; M. Kind ¹ ; ¹ Karlsruhe Institute of Technology (KIT), Karlsruhe/D	
15:50	Discussion with speakers	
16:05	Short Break	
Plenary Lecture		Virtual Room 1
<i>Chair: A. Seidel-Morgenstern, Max Planck Institute for Dynamics of Complex Technical Systems Magdeburg & Otto von Guericke University Magdeburg/D</i>		
16:15	PLENARY LECTURE Modeling, sensing, design and control of crystallizing proteins R. Braatz ¹ ; ¹ Massachusetts Institute of Technology, Cambridge/USA	
17:00	End of second day	

Tuesday, 31 August 2021

Separation of Enantiomers II		Virtual Room 2
<i>Chair: M. Mazzotti, ETH Zurich/CH</i>		
08:30	Modeling crystallization-based deracemization techniques: guidelines for selecting a favorable process for production B. Bodák ¹ ; M. Mazzotti ¹ ; ¹ ETH Zurich/CH	
08:50	Preferential Crystallization of Glutamic Acid Associated by Polymorphism K. Funakoshi ¹ ; S. Naito ¹ ; K. Hayashi ¹ ; ¹ National Institute of Technology, Suzuka College, Suzuka/J	
09:10	Additive-assisted Preferential Crystallization of Racemic Component: A Case of Norvaline J. Sun ¹ ; Y. Wang ¹ ; Z. Gao ¹ ; W. Tang ¹ ; J. Gong ¹ ; ¹ Tiangjin University, Tianjin/CN	
09:30	Preferential Crystallization of the API Guaifenesin in a fluidized bed crystallizer: Seeding strategy development F. Cascella ¹ ; J. Gänsch ² ; A. Seidel-Morgenstern ¹ ; H. Lorenz ² ; ¹ Max-Planck-Institut für Dynamik komplexer technischer Systeme & Otto-von-Guericke-Universität, Magdeburg/D; ² Max Planck Institut für Dynamik komplexer technischer Systeme, Magdeburg/D	
09:50	Discussion with speakers	
10:10	Coffee Break	
10:30	Poster Session II	
12:00	Lunch Break	
Plenary and Keynote Lectures		Virtual Room 1
<i>Chair: R. Geertman, Janssen R&D BE, Beerse/B</i>		
12:45	PLENARY LECTURE Developments in large scale industrial crystallization R. Buchfink ¹ ; C. Melches ¹ ; H. Plate ¹ ; ¹ GEA Messo GmbH, Duisburg/D	
<i>Chair: A. Zwijnenburg, Nouryon Industrial Chemicals - Salt, Deventer/NL</i>		
13:25	KEYNOTE LECTURE An empirical modelling approach of layer crystallization supercharging strategies E. Rigaut ¹ ; E. Temmel ² ; M. Stepanski ¹ ; ¹ Sulzer Chemtech, Winterthur/CH; ² Sulzer Chemtech, Allschwil/CH	
13:50	KEYNOTE LECTURE Pharmaceutical cocrystals: from screening to process development and pre-formulation A. Chow ¹ ; ¹ Agency for Science, Technology & Research (A*STAR), Singapore/SGP	
14:15	Discussion with speakers	
14:30	Coffee Break	
Continuous Crystallization		Virtual Room 2
<i>Chair: Z. Nagy, Loughborough University/UK & Purdue University/USA</i>		
14:50	Development of a Continuous Crystallisation Process in a Stirred-Tank Cascade through Process Analytical Technology Sensors N. Rey ¹ ; P. Riedlberger ¹ ; ¹ Institute of Chemistry and Biotechnology, Zurich University of Applied Sciences (ZHAW), Wädenswil/CH	
15:10	Development of continuous crystallization technologies for direct processing of a flow reaction mixture K. Tacsí ¹ ; Z. Nagy ¹ ; G. Marosi ¹ ; H. Pataki ¹ ; ¹ Budapest University of Technology and Economics (BME), Budapest/H	
15:30	Continuous racemate resolution in coupled fluidized bed crystallizers: Experimental parametric study J. Gänsch ¹ ; E. Temmel ² ; H. Lorenz ¹ ; A. Seidel-Morgenstern ³ ; ¹ Max Planck Institute for Dynamics Complex Technical Systems, Magdeburg/D; ² Sulzer Chemtech Ltd, Allschwil/CH; ³ Otto von Guericke University, Magdeburg/D	
15:50	Discussion with speakers	
16:05	Short Break	
Plenary Lecture		Virtual Room 1
<i>Chair: A. Seidel-Morgenstern, Max Planck Institute for Dynamics of Complex Technical Systems Magdeburg & Otto von Guericke University Magdeburg/D</i>		
16:15	PLENARY LECTURE Modeling, sensing, design and control of crystallizing proteins R. Braatz ¹ ; ¹ Massachusetts Institute of Technology, Cambridge/USA	
17:00	End of second day	

Tuesday, 31 August 2021

Industrial Applications I		Virtual Room 3
<i>Chair: P. Carvin, Solvay, Lyon/F</i>		
08:30	In-line monitoring of sulphate precipitation behavior in industrial crystallizers J. Westerink ¹ ; W. Barnard ¹ ; J. Pek ¹ ; A. Soare ¹ ; A. Schokker ¹ ; <u>A. Zwijnenburg</u> ¹ ; ¹ Nouryon, Deventer/NL	
08:50	Passive Acoustic Emission for Crystallization <u>J. Gebauer</u> ¹ ; ¹ Bayer AG, Leverkusen/D	
09:10	Design, development and scale-up of a skid-based selective dissolution apparatus using liquid cyclonic classifiers and heat exchangers for tailoring crystalline product attributes and crystallization process intensification <u>A. Collas</u> ¹ ; ¹ Janssen Research & Development, Beerse/B	
09:30	Polymorphic Control and Scale-up Strategies for Antisolvent Crystallization by Three Different Feedback Controls <u>I. Østergaard</u> ¹ ; B. Szilagyi ² ; Heidi Lopez de Diego ³ ; Zoltan K. Nagy ² ; Haiyan Qu ¹ ; ¹ University of Southern Denmark, Odense/DK; ² Purdue University, West Lafayette, Indiana/USA; ³ Lundbeck A/S, Copenhagen/DK	
09:50	Discussion with speakers	
10:10	Coffee Break	
10:30	Poster Session II	
12:00	Lunch Break	
Plenary and Keynote Lectures		Virtual Room 1
<i>Chair: R. Geertman, Janssen R&D BE, Beerse/B</i>		
12:45	PLENARY LECTURE Developments in large scale industrial crystallization R. Buchfink ¹ ; <u>C. Melches</u> ¹ ; H. Plate ¹ ; ¹ GEA Messo GmbH, Duisburg/D	
<i>Chair: A. Zwijnenburg, Nouryon Industrial Chemicals - Salt, Deventer/NL</i>		
13:25	KEYNOTE LECTURE An empirical modelling approach of layer crystallization supercharging strategies <u>E. Rigaut</u> ¹ ; E. Temmel ² ; M. Stepanski ¹ ; ¹ Sulzer Chemtech, Winterthur/CH; ² Sulzer Chemtech, Allschwil/CH	
13:50	KEYNOTE LECTURE Pharmaceutical cocrystals: from screening to process development and pre-formulation <u>A. Chow</u> ¹ ; ¹ Agency for Science, Technology & Research (A*STAR), Singapore/SGP	
14:15	Discussion with speakers	
14:30	Coffee Break	
Industrial Applications II		Virtual Room 3
<i>Chair: M. Lee, GlaxoSmithKline, Stevenage, Hertfordshire/UK</i>		
14:50	Development of a Continuous Crystallization with Periodic Wet Milling for Particle Size Control <u>C. Burcham</u> ¹ ; F. Calado ² ; N. Mitchell ² ; S. Myers ¹ ; V. Svoboda ³ ; ¹ Eli Lilly and Company, Indianapolis/USA; ² Process Systems Enterprise, London/UK; ³ Pfizer Inc. Worldwide Research and Development, Sandwich/UK	
15:10	Kinetic Modelling & In-Silico Parametric Analysis of Impurity Inclusion in the Crystallisation of a Pharmaceutical Molecule <u>H. Yao</u> ⁴ ; G. Taylor ¹ ; <u>B. Williams</u> ² ; N. Mitchell ² ; R. Yule ³ ; ¹ GSK, Stevenage/UK; ² PSE - A Siemens Business, London/UK; ³ GSK, Upper Providence/USA; ⁴ GlaxoSmithKline, Colledgeville/USA	
15:30	Comparison of One Dimensional and Two Dimensional Population Balance Models of a Crystallization Process for a Needle Shaped API <u>T. Rosenbaum</u> ¹ ; V. Mbachu ¹ ; N. Mitchell ² ; J. Gamble ³ ; P. Cho ¹ ; J. Engstrom ¹ ; ¹ Bristol-Myers Squibb, New Brunswick/USA; ² Process Systems Enterprise Limited, London/UK; ³ Bristol-Myers Squibb, Moreton/UK	
15:50	Discussion with speakers	
16:05	Short Break	
Plenary Lecture		Virtual Room 1
<i>Chair: A. Seidel-Morgenstern, Max Planck Institute for Dynamics of Complex Technical Systems Magdeburg & Otto von Guericke University Magdeburg/D</i>		
16:15	PLENARY LECTURE Modeling, sensing, design and control of crystallizing proteins <u>R. Braatz</u> ¹ ; ¹ Massachusetts Institute of Technology, Cambridge/USA	
17:00	End of second day	

Wednesday, 1 September 2021

Modeling		Virtual Room 1
<i>Chair: D. Marchisio, Politecnico di Torino, Turin/I</i>		
08:30	Mathematical optimization of partially seeded cooling crystallization accompanied by agglomeration and breakage of crystals J. Unno ¹ ; I. Hirasawa ¹ ; ¹ Waseda University, Tokyo/J	
08:50	Separation of Solid Solutions Using Counter-Current Crystallization V. Tenberg ¹ ; S. Münzberg ¹ ; M. Sadeghi ¹ ; H. Lorenz ¹ ; A. Seidel-Morgenstern ² ; ¹ MPI for Dynamics of Complex Technical Systems, Magdeburg/D; ² Otto von Guericke University / MPI for Dynamics of Complex Technical Systems, Magdeburg/D	
09:10	Morphological Population Balance Modelling of Crystallisation Processes with Heating and Cooling Cycles C. Ma ¹ ; A. Rizvi ¹ ; T. Izumi ² ; K. Roberts ¹ ; ¹ University of Leeds/UK; ² Pfizer R&D UK Limited, Sandwich, Kent /UK	
09:30	Streamlining an Early Phase Crystallisation Development using In-Silico Predictive Modelling and Raman Spectroscopy M. Ukrainczyk ¹ ; J. Zeglinski ¹ ; B. Glennon ¹ ; R. Vanierschot ² ; A. Collas ² ; ¹ APC Ltd., Dublin/IRL; ² Janssen Pharmaceuticals, Beerse/B	
09:50	Discussion with speakers	
10:10	Coffee Break	
10:30	Poster Session III	
12:00	Lunch Break	
Plenary and Keynote Lectures		Virtual Room 1
<i>Chair: C. Melches, GEA Messo GmbH, Duisburg/D</i>		
12:45	PLENARY LECTURE Recovery of critical metals from battery waste by leaching and precipitation processes B. Biscans ¹ ; ¹ University of Toulouse, CNRS, INP, UPS, Toulouse/F	
<i>Chair: M. Stepanski, Sulzer Chemtech Ltd, Winterthur/CH</i>		
13:25	KEYNOTE LECTURE Development of a Modelling Framework for the Co-Precipitation of NMC Hydroxide as Precursor for Lithium Battery Cathodes M. Shiea ¹ ; M. Para ¹ ; G. Tronci ¹ ; A. Buffo ¹ ; G. Boccardo ¹ ; D. Marchisio ¹ ; ¹ Politecnico di Torino, Turin/I	
13:50	KEYNOTE LECTURE Combining reaction with crystallization for process improvement and intensification in continuous manufacturing of antibiotics H. Salami ¹ ; M. McDonald ¹ ; P. Harris ¹ ; C. Lagerman ¹ ; M. Grover ¹ ; A. Bommarius ¹ ; R. Rousseau ¹ ; ¹ Georgia Institute of Technology, Atlanta/USA	
14:15	Discussion with speakers	
14:30	Coffee Break	
Crystalline Phase Behaviour		Virtual Room 1
<i>Chair: J. Gómez Morales, CSIC - University of Granada/E</i>		
14:50	A plastically bent crystal: the correlation between crystal structure and mechanical properties Y. Liu ¹ ; S. Wu ¹ ; J. Gong ¹ ; ¹ Tianjin University, Tianjin/CN	
15:10	Organic Mesocrystals: A new strategy to enhance the drug dissolution R. Mani ¹ ; M. Louhi-Kultanen ¹ ; ¹ Aalto University School of Chemical Engineering, Espoo/FIN	
15:30	Can surfactant self-assemblies be used to control polymorphism? F. Marques Penha ¹ ; F. Ibis ² ; A. Gopalan ² ; J. Meijlink ² ; H. Eral ² ; ¹ KTH Royal Institute of Technology, Stockholm/S; ² Delft University of Technology, Delft/NL	
15:50	Discussion with speakers	
16:05	Short Break	
Plenary Lecture		Virtual Room 1
<i>Chair: M. Rauls, BASF SE, Ludwigshafen/D</i>		
16:15	PLENARY LECTURE Industrial crystallization – establishing solid state properties for both downstream processing and product performance D. Green ¹ ; ¹ GlaxoSmithKline, Collegeville/USA	
17:00	End of third day	

Wednesday, 1 September 2021

Reactive Crystallization		Virtual Room 2
<i>Chair: B. Biscans, University of Toulouse, CNRS, INP, UPS, Toulouse/F</i>		
08:30	Crystallization of (lanthanide, calcium) phosphate nanophosphors J. Gómez-Morales ¹ ; R. Fernández-Penas ¹ ; C. Verdugo-Escamilla ¹ ; D. Choquesillo-Lazarte ¹ ; C. Drouet ² ; F. Oltolina ³ ; M. Prat ³ ; M. Iafisco ⁴ ; J. Fernández-Sánchez ⁵ ; ¹ Instituto Andaluz de Ciencias de la Tierra, Consejo Superior de Investigaciones Científicas, Armilla/E; ² CNRS / University of Toulouse/F; ³ University of Piemonte Orientale, Novara/I; ⁴ CNR - National Research Council of Italy, Faenza/I; ⁵ University of Granada/E	
08:50	Control of Reaction Crystallization of Organic Compounds Considering with Supersaturation Profile H. Takiyama ¹ ; ¹ Tokyo University of Agriculture and Technology, Tokyo/J	
09:10	A compartmental-based approach for the modelling of a vortex precipitation reactor for nuclear energy applications C. Ruiz Vasquez ¹ ; N. Lebaz ² ; D. Mangin ² ; M. Bertrand ³ ; E. Saikali ⁴ ; M. Rodio ⁴ ; G. Bois ⁴ ; U. Bieder ⁴ ; ¹ CEA Marcoule, Villeurbanne, France/F; ² LAGEPP, Université de Lyon, CNRS UMR5007, Lyon/F; ³ CEA, DEN, DMRC, Université Montpellier, Marcoule/F; ⁴ CEA, DEN, STMF, Saclay/F	
09:30	Model-based design and control of precipitation processes in industrial applications L. Metzger ¹ ; M. Kespe ¹ ; T. Beierling ¹ ; M. Voges ¹ ; ¹ BASF SE, Ludwigshafen/D	
09:50	Discussion with speakers	
10:10	Coffee Break	
10:30	Poster Session III	
12:00	Lunch Break	
Plenary and Keynote Lectures		Virtual Room 1
<i>Chair: C. Melches, GEA Messo GmbH, Duisburg/D</i>		
12:45	PLENARY LECTURE Recovery of critical metals from battery waste by leaching and precipitation processes B. Biscans ¹ ; ¹ University of Toulouse, CNRS, INP, UPS, Toulouse/F	
<i>Chair: M. Stepanski, Sulzer Chemtech Ltd, Winterthur/CH</i>		
13:25	KEYNOTE LECTURE Development of a Modelling Framework for the Co-Precipitation of NMC Hydroxide as Precursor for Lithium Battery Cathodes M. Shiea ¹ ; M. Para ¹ ; G. Tronci ¹ ; A. Buffo ¹ ; G. Boccardo ¹ ; D. Marchisio ¹ ; ¹ Politecnico di Torino, Turin/I	
13:50	KEYNOTE LECTURE Combining reaction with crystallization for process improvement and intensification in continuous manufacturing of antibiotics H. Salami ¹ ; M. McDonald ¹ ; P. Harris ¹ ; C. Lagerman ¹ ; M. Grover ¹ ; A. Bommarius ¹ ; R. Rousseau ¹ ; ¹ Georgia Institute of Technology, Atlanta/USA	
14:15	Discussion with speakers	
14:30	Coffee Break	
Battery Materials		Virtual Room 2
<i>Chair: M. Rauls, BASF SE, Ludwigshafen/D</i>		
14:50	Coprecipitation of Ni_xMn_yCo_{1-x-y}(OH)₂ as precursor for ion lithium batteries: influence of mixing and operating conditions M. Para ¹ ; M. Alidoost ¹ ; M. Shiea ¹ ; A. Buffo ¹ ; G. Boccardo ¹ ; R. Pisano ¹ ; A. Barresi ¹ ; D. Marchisio ¹ ; ¹ Politecnico di Torino/I	
15:10	Impact of Sulphate Intercalation on the Morphology of Co-Precipitated Battery Material Precursors R. Berk ¹ ; L. Metzger ¹ ; T. Beierling ¹ ; M. Rauls ¹ ; ¹ BASF SE Ludwigshafen/D	
15:30	Recycling process of lithium from batteries by Li₂CO₃ precipitation M. Le Page Mostefa ¹ ; C. Baumann ¹ ; H. Muhr ¹ ; ¹ LRGP - UMR 7274 CNRS, Nancy/F	
15:50	Discussion with speakers	
16:05	Short Break	
Plenary Lecture		Virtual Room 1
<i>Chair: M. Rauls, BASF SE, Ludwigshafen/D</i>		
16:15	PLENARY LECTURE Industrial crystallization – establishing solid state properties for both downstream processing and product performance D. Green ¹ ; ¹ GlaxoSmithKline, Colledgeville/USA	
17:00	End of third day	

Wednesday, 1 September 2021

Contributions to Sustainability		Virtual Room 3
<i>Chair: A. Lewis, University of Cape Town/ZA</i>		
08:30	Selective crystallisation of magnesium and calcium hydroxides from industrial waste brines: a pilot study F. Vassallo ¹ ; D. La Corte ¹ ; N. Cancilla ¹ ; M. Bevacqua ² ; A. Tamburini ¹ ; A. Cipollina ¹ ; G. Micale ¹ ; ¹ University of Palermo/I; ² ResourSEAs Srl, Palermo/I	
08:50	Investigating the effect of surface properties on ice scaling in Eutectic Freeze Crystallization L. Motsepe ¹ ; ¹ University of Cape Town/ZA	
09:10	Experimental review of a scraped-stirred crystallizer design for Eutectic Freeze Crystallization M. Rodriguez Pascual ¹ ; D. Xevgenos ² ; ¹ Water Energy Intelligence, Schiedam/NL; ² TU Delft/NL	
09:30	A sub-zero crystallization process for the recovery of lactose R. Halfwerk ¹ ; D. Yntema ² ; J. Van Spronsen ³ ; A. Van der Padt ⁴ ; ¹ Wageningen University/Wetsus European Centre of Excellence for Sustainable Water Technology, Wageningen/NL; ² Wetsus European Centre of Excellence for Sustainable Water Technology, Leeuwarden/NL; ³ Cool Separations BV, Portugal/NL; ⁴ FrieslandCampina/Wageningen University, Amersfoort /NL	
09:50	Discussion with speakers	
10:10	Coffee Break	
10:30	Poster Session III	
12:00	Lunch Break	
Plenary and Keynote Lectures		Virtual Room 1
<i>Chair: C. Melches, GEA Messo GmbH, Duisburg/D</i>		
12:45	PLENARY LECTURE Recovery of critical metals from battery waste by leaching and precipitation processes B. Biscans ¹ ; ¹ University of Toulouse, CNRS, INP, UPS, Toulouse/F	
<i>Chair: M. Stepanski, Sulzer Chemtech Ltd, Winterthur/CH</i>		
13:25	KEYNOTE LECTURE Development of a Modelling Framework for the Co-Precipitation of NMC Hydroxide as Precursor for Lithium Battery Cathodes M. Shiea ¹ ; M. Para ¹ ; G. Tronci ¹ ; A. Buffo ¹ ; G. Boccardo ¹ ; D. Marchisio ¹ ; ¹ Politecnico di Torino, Turin/I	
13:50	KEYNOTE LECTURE Combining reaction with crystallization for process improvement and intensification in continuous manufacturing of antibiotics H. Salami ¹ ; M. McDonald ¹ ; P. Harris ¹ ; C. Lagerman ¹ ; M. Grover ¹ ; A. Bommarius ¹ ; R. Rousseau ¹ ; ¹ Georgia Institute of Technology, Atlanta/USA	
14:15	Discussion with speakers	
14:30	Coffee Break	
Integrated Processes II		Virtual Room 3
<i>Chair: B. Glennon, University College Dublin/IRL</i>		
14:50	Integrated Process Design of Continuous Solid-Liquid Separation, Washing, and Drying for Crystal Suspensions with Varying Crystal Shapes C. Steenweg ¹ ; J. Habicht ¹ ; G. Schembecker ¹ ; K. Wohlgemuth ¹ ; ¹ TU Dortmund University, Dortmund/D	
15:10	Utilization of Quality-by-Control for rapid process design of agrochemical crystallization. W. Wu ¹ ; C. Chappelow ² ; M. Kodam ³ ; P. Larsen ³ ; P. McGough ³ ; J. Patton ² ; A. Shinkle ² ; Z. Nagy ¹ ; ¹ Purdue University, West Lafayette/USA; ² Corteva Agriscience, Midland/USA; ³ Corteva Agriscience, Indianapolis/USA	
15:30	Digital Design of crystallization process: Application of a mechanistic morphological crystallizer model to improve powder flowability via aspect ratio reduction N. Mitchell ¹ ; S. Douieb ² ; F. Calado ¹ ; U. Cocchini ² ; P. Marzoli ¹ ; E. Hadjittofis ² ; J. Uyttersprot ² ; N. Carly ² ; J. Mantanus ² ; ¹ PSE - A Siemens Business, London/UK; ² UCB Pharma SA, Anderlecht/B	
15:50	Discussion with speakers	
16:05	Short Break	
Plenary Lecture		Virtual Room 1
<i>Chair: M. Rauls, BASF SE, Ludwigshafen/D</i>		
16:15	PLENARY LECTURE Industrial crystallization – establishing solid state properties for both downstream processing and product performance D. Green ¹ ; ¹ GlaxoSmithKline, Collegeville/USA	
17:00	End of third day	

Thursday, 2 September 2021

Microfluidic Techniques		Virtual Room 1
<i>Chair: K. Wohlgemuth, TU Dortmund/D</i>		
08:30	Nucleation kinetics of Calcium Oxalate Monohydrate as a function of supersaturation and pH quantified with droplet microfluidics <u>F. Ibis</u> ¹ ; T. Wang Yu ¹ ; F. Marques Penha ¹ ; D. Ganguly ¹ ; M. Alhaji Nuhu ¹ ; A. van der Heijden ¹ ; H. Kramer ¹ ; H. Eral ¹ ; ¹ TU Delft/NL	
08:50	Microfluidics platform for polymorph screening directly from powder <u>G. Peybernes</u> ¹ ; R. Grossier ¹ ; F. Villard ² ; P. Letellier ² ; N. Candoni ¹ ; S. Veessler ¹ ; ¹ Aix-Marseille University & CNRS, CINaM, Marseille/F; ² Technologie Servier, Orléans/F	
09:10	Nucleation in Sessile Microdroplet Arrays: Accounting for Diffusive Interactions <u>R. Cedeno</u> ¹ ; R. Grossier ² ; A. Flood ³ ; N. Candoni ⁴ ; S. Veessler ⁴ ; ¹ CNRS - Aix Marseille Université / Vidyasirimedhi Institute of Science and Technology (VISTEC), Marseille/F; ² CNRS, Marseille/F; ³ Vidyasirimedhi Institute of Science and Technology (VISTEC), Rayong/T; ⁴ CNRS - Aix-Marseille University, Marseille/F	
09:30	Embedded droplet printing for pharmaceutical drug particle synthesis <u>A. Nelson</u> ¹ ; J. Xie ² ; S. Khan ² ; P. Doyle ³ ; ¹ Singapore-MIT Alliance for Research and Technology, Singapore/SGP; ² National University of Singapore, Singapore/SGP; ³ Massachusetts Institute of Technology; Singapore-MIT Alliance for Research and Technology, Cambridge/USA	
09:50	Discussion with speakers	
10:10	Coffee Break	
10:30	Poster Session IV	
11:30	Lunch Break	

Plenary and Keynote Lectures		Virtual Room 1
<i>Chair: H. Lorenz, Max Planck Institute for Dynamics of Complex Technical Systems & Otto von Guericke University, Magdeburg/D</i>		
12:15	PLENARY LECTURE Nucleation theories, 80 years research on nucleation <u>H. Cölfen</u> ¹ ; ¹ Department of Physical Chemistry, University of Konstanz/D	
12:55	KEYNOTE LECTURE Understanding the Solutions You Crystallise from: The Molecular Basis of Co-solvency and Conformational Changes by X-ray Pair Distribution Function Measurements and Modelling <u>A. Pallipurath</u> ¹ ; B. Evans ² ; L. Al-Madhagi ² ; A. Pugejs ² ; S. Schroeder ² ; ¹ University of of Leeds/UK; ² School of Chemical and Process Engineering, University of Leeds/UK	
<i>Chair: M. Mazzotti; ETH Zurich/CH</i>		
13:20	EFCE PRIZE AWARD LECTURE 2020 / 2021 A Dual Projection Imaging System to Characterize Crystallization Processes: Design and Applications A.K. Rajagopalan, ETH Zurich/CH	
13:45	Discussion with speakers	
14:00	Closing & Announcement 22nd ISIC	
14:15	End of lecture programme	

Thursday, 2 September 2021

14:30 – 17:30	TUTORIAL C
Modeling, Monitoring and Control of Crystallization Systems Z.K. Nagy ¹ ; R. Braatz ² ; E. Simone ³ ; N. Yazdanpanah ⁴ ; B. Szilagy ⁵ ; ¹ Loughborough University, Leicestershire/UK and Purdue University/USA; ² MIT, USA; ³ Leeds University/UK; ⁴ Procegen/USA; ⁵ Purdue University/USA	

Thursday, 2 September 2021

Lectures to Honor Gerda v. Rosmalen & Special Techniques		Virtual Room 2
<i>Chairs: J. ter Horst, Université de Rouen Normandie, Mont-Saint-Aignan/F; H. Wei, Tianjin University of Science and Technology/PRC</i>		
08:30	Unique approaches to problem solving in Industrial Crystallization: Remembering Gerda van Rosmalen A. Lewis ¹ ; ¹ University of Cape Town/ZA	
08:50	Steering crystallization with light, flow and soft matter B. Eral ¹ ; ¹ Delft University of Technology/NL	
09:10	Impurities and oiling-out brought us better results K. Tanaka ¹ ; ¹ CHUGAI PHARMACEUTICAL. CO., LTD., Kita-ku, Tokyo/J	
09:30	An efficient strategy for manipulating the crystal morphology of active pharmaceutical ingredients in stirred systems N. Ramos ¹ ; R. Diodone ² ; P. Hidber ² ; M. Kind ¹ ; ¹ Karlsruhe Institut of Technology, Karlsruhe/D; ² F. Hoffmann-La Roche AG, Basel/CH	
09:50	Discussion with speakers	
10:10	Coffee Break	
10:30	Poster Session IV	
11:30	Lunch Break	

Plenary and Keynote Lectures		Virtual Room 1
<i>Chair: H. Lorenz, Max Planck Institute for Dynamics of Complex Technical Systems & Otto von Guericke University, Magdeburg/D</i>		
12:15	PLENARY LECTURE Nucleation theories, 80 years research on nucleation H. Cölfen ¹ ; ¹ Department of Physical Chemistry, University of Konstanz/D	
12:55	KEYNOTE LECTURE Understanding the Solutions You Crystallise from: The Molecular Basis of Co-solvency and Conformational Changes by X-ray Pair Distribution Function Measurements and Modelling A. Pallipurath ¹ ; B. Evans ² ; L. Al-Madhagi ² ; A. Pugejs ² ; S. Schroeder ² ; ¹ University of Leeds/UK; ² School of Chemical and Process Engineering, University of Leeds/UK	
<i>Chair: M. Mazzotti; ETH Zurich/CH</i>		
13:20	EFCE PRIZE AWARD LECTURE 2020 / 2021 A Dual Projection Imaging System to Characterize Crystallization Processes: Design and Applications A.K. Rajagopalan, ETH Zurich/CH	
13:45	Discussion with speakers	
14:00	Closing & Announcement 22nd ISIC	
14:15	End of lecture programme	

Thursday, 2 September 2021

14:30 – 17:30	TUTORIAL C
Modeling, Monitoring and Control of Crystallization Systems Z.K. Nagy ¹ ; R. Braatz ² ; E. Simone ³ ; N. Yazdanpanah ⁴ ; B. Szilagyi ⁵ ; ¹ Loughborough University, Leicestershire/UK and Purdue University/USA; ² MIT, USA; ³ Leeds University/UK; ⁴ Procegen/USA; ⁵ Purdue University/USA	

Thursday, 2 September 2021

Special Techniques		Virtual Room 3
<i>Chair: A. Chow, Agency for Science, Technology & Research (A*STAR), Singapore/SGP</i>		
08:30	Microfluidic-assisted controlled spherical crystallization of Naproxen-Eudragit E100 microparticles S. Shikha ¹ ; S. Khan ² ; P. Doyle ³ ; ¹ Singapore-MIT Alliance for Research and Technology, Singapore/SGP; ² National University of Singapore/SGP; ³ Massachusetts Institute of Technology (MIT); Singapore-MIT Alliance for Research and Technology, Cambridge/USA	
08:50	Protein Crystallisation with Gas Bubble Templates W. Tian ¹ ; C. Rielly ¹ ; H. Yang ¹ ; ¹ Loughborough University, Loughborough/UK	
09:10	Pickering Emulsion Assisted Spherical Crystallization of Ibuprofen J. Wang ¹ ; W. Cao ¹ ; L. Zhu ¹ ; ¹ Zhejiang University of Technology, Hangzhou/CN	
09:30	The integration of membrane emulsification and cooling crystallization of glycine S. Kwon ¹ ; K. Mathew Thomas ¹ ; R. Lakerveld ¹ ; ¹ The Hong Kong University of Science and Technology, Clear Water Bay, Kowloon/HK	
09:50	Discussion with speakers	
10:10	Coffee Break	
10:30	Poster Session IV	
11:30	Lunch Break	

Plenary and Keynote Lectures		Virtual Room 1
<i>Chair: H. Lorenz, Max Planck Institute for Dynamics of Complex Technical Systems & Otto von Guericke University, Magdeburg/D</i>		
12:15	PLENARY LECTURE Nucleation theories, 80 years research on nucleation H. Cölfen ¹ ; ¹ Department of Physical Chemistry, University of Konstanz/D	
12:55	KEYNOTE LECTURE Understanding the Solutions You Crystallise from: The Molecular Basis of Co-solvency and Conformational Changes by X-ray Pair Distribution Function Measurements and Modelling A. Pallipurath ¹ ; B. Evans ² ; L. Al-Madhagi ² ; A. Pugejs ² ; S. Schroeder ² ; ¹ University of of Leeds/UK; ² School of Chemical and Process Engineering, University of Leeds/UK	
<i>Chair: M. Mazzotti; ETH Zurich/CH</i>		
13:20	EFCE PRIZE AWARD LECTURE 2020 / 2021 A Dual Projection Imaging System to Characterize Crystallization Processes: Design and Applications A.K. Rajagopalan, ETH Zurich/CH	
13:45	Discussion with speakers	
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Thursday, 2 September 2021

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Modeling, Monitoring and Control of Crystallization Systems Z.K. Nagy ¹ ; R. Braatz ² ; E. Simone ³ ; N. Yazdanpanah ⁴ ; B. Szilagyi ⁵ ; ¹ Loughborough University, Leicestershire/UK and Purdue University/USA; ² MIT, USA; ³ Leeds University/UK; ⁴ Procegen/USA; ⁵ Purdue University/USA	

POSTER SESSIONS

The poster authors should be ready for poster discussions during the poster sessions. Following topics will be discussed on following dates:

Monday, 30 August 2021

16:25 – 17:30

POSTER SESSION I

Developments in Large Scale Industrial Crystallization

P 1.01 – P 1.10

Contributions of Crystallization to Sustainability

P 2.01 – P 2.08

Tuesday, 31 August 2021

10:30 – 12:00

POSTER SESSION II

Fundamentals of Crystallization

P 3.01 – P 3.49

Wednesday, 1 September 2021

10:30 – 12:00

POSTER SESSION III

Crystallization & Precipitation in Fine Chemical, Specialty & Life-Science Industries

P 4.01 – P 4.35

Thursday, 2 September 2021

10:30 – 11:30

POSTER SESSION IV

Integrated Process Design: Crystallization Process Design in the Industrial Process Chain

P 5.01 – P 5.15

POSTER SESSION I

Developments in Large Scale Industrial Crystallization

Posters will be discussed on Monday, 30 August 2021

16:25 – 17:30

- P 1.01 **Crystallization process development using Secoy's Crystallization Technology: from lab scale units to a full scale process unit**
B. Rimez¹; ¹ Secoya technologies, Louvain-la-Neuve/B
- P 1.02 **Population Balance Modeling of Cooling-Antisolvent Crystallization to Derisk Tech-Transfer**
T. Rosenbaum¹; L. Tan¹; N. Mitchell²; M. Dummeldinger¹; J. Engstrom¹; ¹ Bristol-Myers Squibb, New Brunswick/USA; ² Process Systems Enterprise Limited, London/UK
- P 1.04 **Study of scaling in a plate heat exchanger**
N. Kamar¹; M. Le Page Mostefa¹; H. Muhr¹; P. Jost²; ¹ Laboratoire Réaction et Génie des Procédés, Université de Lorraine, Nancy/F; ² Sofchem, Rueil Malmaison /F
- P 1.05 **Batch crystallization of xylitol by cooling, evaporation and anti-solvent addition**
A. Zaykovskaya¹; E. Temmel²; M. Stepanski³; B. Gevers Deynoot⁴; E. de Jong⁴; M. Louhi-Kultanen⁵; ¹ Aalto University School of Chemical Engineering, Espoo/FIN; ² Sulzer Chemtech Ltd, Allschwil/CH; ³ Sulzer Chemtech Ltd, Winterthur/CH; ⁴ Avantium, Amsterdam/NL; ⁵ Aalto University, Espoo/FIN
- P 1.06 **New developments in impeller design for solid-liquid applications**
B. Nienhaus¹; ¹ EKATO Rühr- und Mischtechnik GmbH, Schopfheim/D
- P 1.07 **A 3D-Printed Low Pressure-Drop Plug-Flow Crystallizer for Protein Crystallization**
B. Nyande¹; K. Mathew Thomas¹; R. Lakerveld¹; ¹ The Hong Kong University of Science and Technology, Hong Kong/HK
- P 1.08 **Ice scaling formation on scraped heat exchanger surfaces during melt/cooling crystallization**
M. Rodriguez Pascual¹; D. Xevgenos²; ¹ Delft University of Technology, Delft/NL; ² TU Delft/NL
- P 1.09 **Bullet-Proofing Doravirine (MK-1439) Starting Material Supply: Rapid Identification and Response to a New Polymorph of Ethyl Ester**
P. Larpent¹; L. Codan¹; J. Schoell¹; L. Iuzzolino²; M. Tan²; J. Newman²; A. Lee²; ¹ MSD Werthenstein BioPharma, Schachen/CH; ² Merck & Co. Inc., Rahway/USA
- P 1.10 **A novel image analysis technique for 2D characterization of overlapping needle like crystals**
P. Neoptolemos¹; ¹ The University of Manchester/UK

POSTER SESSION I

Contributions of Crystallization to Sustainability

Posters will be discussed on Monday, 30 August 2021

16:25 – 17:30

- P 2.01 **CaCO₃ precipitation through the carbonation route towards cement industry circular economy**
F. Liendo Castillo¹; F. Deorsola¹; S. Bensaid¹; ¹ Politecnico di Torino, Turin/I
- P 2.02 **-CODA- The Carbon-Negative Soda Ash Project**
 H. Lorenz¹; S. Ghaffari¹; C. Eisenhut²; P. Schulze³; ¹ Max Planck Institut für Dynamik komplexer technischer Systeme, Magdeburg/D; ² CIECH Soda Deutschland GmbH & Co. KG, Staßfurt/D; ³ SchPrEngCo- Scientific Chemical Process Engineering Consultancy, Magdeburg/D
- P 2.03 **Melt Crystallization of 2,4-Dinitrochlorobenzene: Crystal Growth and Sweating Process Evaluation**
S. Jia¹; J. Gong¹; Z. Gao¹; J. Wang¹; ¹ Tianjin University/CN
- P 2.04 **CFD-PBM simulation of Mg(OH)₂ precipitation from saltwork brine**
A. Raponi¹; A. Buffo¹; G. Boccardo¹; M. Vanni¹; D. Marchisio¹; G. Montalbano¹; G. Battaglia²; S. Romano²; ¹ DISAT – Politecnico di Torino/I; ² Dip. Ingegneria – Università di Palermo/I
- P 2.05 **Towards product separation by cooling crystallization as part of an integrated catalyst recycling process**
A. Seifert¹; A. Laudanski¹; J. Simons¹; T. Seidensticker¹; K. Wohlgemuth¹; ¹ TU Dortmund University, Dortmund/D

- P 2.06 **Understanding Crystallisation in Plant Cuticular Waxes in Relations to Water Permeation through Plant Surfaces**
L. Parameswaran¹; K. Roberts¹; X. Lai¹; N. George²; M. Riederer³; ¹ University of Leeds/UK;
² Syngenta Crop Protection, Jealott's Hill/UK; ³ Julius Maximilians University of Würzburg/D
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- P 2.07 **CFD Study on Heat Transfer in a Layer Melt Crystallizer**
N. Osmanbegovic¹; V. Alopaeus^{1,2}; V. Vuorinen¹; M. Louhi-Kultanen¹; ¹ Aalto University School of Chemical Engineering, Espoo/FIN; ² Aalto University School of Engineering, Espoo/FIN; ² Department of Chemical Engineering, Mid Sweden University, Sundsvall/S
-
- P 2.08 **Synthetic BiOBr/Bi₂S₃/CdS crystalline material and its degradation of dye under visible light**
J. Chen¹; Y. Jin¹; Z. Xing¹; Y. Li¹; J. Han¹; H. Lorenz²; ¹ Hebei University of Technology, Tianjin/CN; ² Max Planck Institute for Dynamics of Complex Technical Systems, Munich/D

POSTER SESSION II

Fundamentals of Crystallization

Posters will be discussed on Tuesday, 31 August 2021

10:30 – 12:00

- P 3.01 **Hierarchical BaCO₃/SiO₂ Biomorphs: Morphological Evolution & Multi-Functional Development**
Y. Chen¹; S. Wang¹; J. Gong¹; ¹ Tianjin University, Tianjin/CN
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- P 3.02 **The development of precipitate characteristics by means of the reactor type and operating conditions**
M. Stec¹; P. Synowiec¹; B. Bunikowska¹; ¹ Silesian University of Technology / Research Network Łukasiewicz, New Chemical Syntheses Institute, Inorganic Chemistry Division "IChN", Gliwice/PL
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- P 3.03 **Crystallization of magnesium sulphate heptahydrate from solutions containing calcium and chlorides**
B. Bunikowska¹; P. Synowiec¹; M. Stec¹; ¹ Silesian University of Technology / Research Network Łukasiewicz, New Chemical Syntheses Institute, Inorganic Chemistry Division "IChN", Gliwice/PL
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- P 3.04 **Simultaneous crystallization in the ternary system NaCl-Na₂SO₄-H₂O**
 A. Sarubbi Lanzotti¹; M. Martins Seckler¹; ¹ University of São Paulo/BR
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- P 3.05 **Thermodynamic based process design for polymers forming different crystalline phases**
 Z. Fan¹; S. Enders²; M. Fischlschweiger¹; ¹ TU Clausthal / Lehrstuhl für Technische Thermodynamik und Energieeffiziente Stoffbehandlung, Clausthal-Zellerfeld/D; ² KIT Institut für Technische Thermodynamik und Kältetechnik, Karlsruhe/D
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- P 3.06 **Growth of crystal faces tracked in 3D**
S. Schiele¹; H. Briesen¹; ¹ TU München, Freising/D
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- P 3.07 **Stratification of multi-component solutions on crystalline substrates**
C. Helfenritter¹; M. Kind¹; ¹ Karlsruhe Institute of Technology (KIT), Karlsruhe/D
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- P 3.08 **Bernoulli offers a solid basis for crystallization**
H. Meldau¹; ¹ ehemals Sulzer Escher Wyss, Hannover/D
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- P 3.09 **Ultrasound-Assisted Crystallization Process Intensification of L-glutamic Acid: Crystal Nucleation and Polymorph Transformation**
C. Fang¹; Z. Gao¹; J. Gong¹; J. Wang¹; ¹ Tianjin University, Tianjin/CN
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- P 3.10 **Controlled Crystallization Process of Potassium Nitrate Solution: Incrustation Phenomenon**
 M. Al-Rashed¹; A. Alenzi¹; A. Mohammad¹; J. Wójcik²; ¹ College of Technological Studies, The Public Authority for Applied Education and Training, Shuwaikh/KWT; ² Silesian University of Technology, Gliwice/PL
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- P 3.11 **Implementation of thermal cycling for the control of crystal morphology and size distribution**
J. Zeglinski¹; M. Ukrainczyk¹; G. Morris¹; B. Glennon¹; ¹ APC Ltd., Dublin/IRL
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- P 3.12 **Thermodynamic description of phase diagrams in solid solution/solvent systems**
M. Sadeghi¹; S. Münzberg¹; V. Tenberg¹; H. Lorenz¹; A. Seidel-Morgenstern²; ¹ Max-Planck-Institut für Dynamik komplexer technischer Systeme, Magdeburg/D; ² Max-Planck-Institut für Dynamik komplexer technischer Systeme & Otto-von-Guericke-Universität Magdeburg, Magdeburg/D
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- P 3.13 **Fluidic Oscillator as a Continuous Crystalliser: Modelling and Validation**
Y. Yu¹; A. Pandit²; V. Ranade¹; ¹ Queen's University Belfast/UK; ² Bernal Institute, University of Limerick, Limerick/IRL

- P 3.14 **Crystallizer geometry optimization applying the process model for the Separation of Enantiomers by Preferential Crystallization**
 N. Huskova¹; M. Mangold²; H. Lorenz³; A. Seidel-Morgenstern³; ¹ Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg/D; ² Technische Hochschule Bingen/D; ³ Max Planck Institute for Dynamics of Complex Technical Systems & Otto von Guericke University, Magdeburg/D
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- P 3.15 **Modeling crystal growth using the lattice Boltzmann method**
 Q. Tan¹; H. Lorenz²; S. Hosseini¹; A. Seidel-Morgenstern²; D. Thévenin¹; ¹ OVGU, Magdeburg, Magdeburg/D; ² Max Planck Institute for Dynamics of Complex Technical Systems (MPI Magdeburg), Magdeburg/D
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- P 3.16 **Strategic Application of Temperature Correction Algorithms for Improved in situ Concentration Monitoring During Cooling Crystallisation**
 M. Chong¹; T. McGlone¹; A. Parrott¹; A. Nordon¹; A. Florence¹; ¹ University of Strathclyde, Glasgow/UK
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- P 3.17 **A novel colorimetric experimental technique for the characterization of metal hydroxides reactive crystallization phenomena**
 S. Romano¹; G. Battaglia¹; A. Tamburini¹; M. Ciofalo¹; A. Cipollina¹; G. Micale¹; ¹ Università degli Studi di Palermo/I
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- P 3.19 **Semi-Batch Evaporation Crystallization for Cobalt Sulfate Recovery**
 J. Zhang¹; A. Said¹; B. Han¹; M. Louhi-Kultanen¹; ¹ Aalto University, Espoo/FIN
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- P 3.20 **Impact of the phase transition phenomenon of a UCST-type thermoresponsive polymers onto the crystallization of inorganic salts**
 E. Wong Munoz¹; M. Lemanowicz¹; A. Mielańczyk¹; K. Kiraga¹; A. Gierczycki¹; ¹ Silesian University of Technology, Gliwice/PL
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- P 3.21 **Time-Resolved X-ray Phase-Contrast Imaging of Continuous Anti-Solvent Crystallisation**
 G. Das¹; A. Pallipurath²; T. Kathyola²; J. Leng²; S. Marathe³; C. Rau³; J. McGinty⁴; R. Miller⁴; J. Sefcik⁴; S. Schroeder²; ¹ School of Chemical and Process Engineering, University of Leeds/UK; ² University of Leeds/UK; ³ Diamond Light Source, Didcot/UK; ⁴ University of Strathclyde/CMAC, Glasgow/UK
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- P 3.22 **Thermodynamics of Co-Crystal Formation: Estimating the Stability of Sulfamethazine Co-Crystals**
 M. Svärd¹; D. Ahuja²; ¹ KTH Royal Institute of Technology, Stockholm/S; ² University of Limerick, Limerick/IRL
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- P 3.23 **Precipitation of calcium oxalate in a multifunctional reactor**
 A. Malysiak¹; S. Musial¹; P. Polak¹; ¹ Silesian University of Technology, Gliwice/PL
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- P 3.24 **Application of image analysis methods to enhance crystal shape identification and face indexing**
 F. Luxenburger¹; E. Elts¹; H. Briesen¹; ¹ Lehrstuhl für Systemverfahrenstechnik, TU München, Freising/D
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- P 3.25 **Effect of solvents on crystal size distribution in ultrasound assisted crystallization of ascorbic acid**
 J. Yadav¹; S. Patel¹; ¹ Indian Institute of Technology Ropar, Ropar/IND
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- P 3.26 **Experimental Investigation of an Integrated Crystallization and Wet-Milling System with Temperature Cycling to Control the Size and Aspect Ratio of Needle-Shaped Pharmaceutical Crystals**
 A. Eren¹; B. Szilágyi¹; J. Quon²; C. Papageorgiou²; Z. Nagy¹; ¹ Purdue University, Lafayette/USA; ² Takeda Pharmaceuticals International Co., Cambridge/USA
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- P 3.27 **Approaches to drying Active Pharmaceutical Ingredients**
 E. Keavney¹; B. Wood²; A. Healy¹; B. Glennon²; ¹ Trinity College Dublin, The University of Dublin/IRL; ² APC Ltd., Dublin/IRL
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- P 3.28 **Reverse antisolvent crystallization using membrane pervaporation: application to L-Glutamic Acid**
 M. Khellaf¹; C. Charcosset¹; D. Mangin¹; E. Chabanon¹; ¹ LAGEPP/University of Claude Bernard Lyon 1, Villeurbanne/F
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- P 3.29 **Model-driven Controller Design for Continuous Crystallisation of α -Lactose Monohydrate**
 J. Johnston¹; C. Brown¹; A. Florence¹; ¹ CMAC/University of Strathclyde, Glasgow/UK
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- P 3.30 **1D and 2-D population balance models applied to mefenamic acid solution crystallisation using gFORMULATE**
 W. Li¹; B. Benyahia¹; C. Rielly¹; ¹ Loughborough University, Loughborough/UK
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- P 3.31 **Microfluidics set-up rapidly measures solubility directly from powder**
 G. Peybernes¹; R. Grossier¹; F. Villard²; P. Letellier²; N. Candoni¹; S. Veester¹; ¹ Aix-Marseille University & CNRS, CINaM, Marseille/F; ² Technologie Servier, Orléans/F

- P 3.32 **Template-assisted protein crystallization in microfluidics**
D. Powell¹; C. Gerard¹; M. Briuglia¹; S. Morais²; D. Lamprou³; J. Salmon²; J. ter Horst¹; ¹ University of Strathclyde/CMAC, Glasgow/UK; ² CNRS, Université de Bordeaux, Institut de Chimie de la Matière Condensée de Bordeaux, Bordeaux/F; ³ Queens University Belfast/UK
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- P 3.33 **Design and validation of a droplet based microfluidic system to study non-photochemical laser induced nucleation**
V. Korede¹; F. Penha²; D. Irimia¹; L. Stam¹; V. Munck¹; A. Heijden¹; H. Kramer¹; H. Eral¹; ¹ Delft University of Technology, Delft/NL; ² KTH Royal Institute of Technology, Stockholm/S
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- P 3.34 **Primary and Secondary Nucleation of Sodium Chloride from Water and Deuterium Oxide**
J. Flannigan¹; M. Haw²; H. Jolliffe³; J. Sefcik¹; ¹ EPSRC Centre for Innovative Manufacturing in Continuous Manufacturing and Crystallisation, c/o Department of Chemical and Process Engineering, University of Strathclyde, Glasgow/UK; ² Department of Chemical and Process Engineering, University of Strathclyde, Glasgow/UK; ³ EPSRC Centre for Innovative Manufacturing in Continuous Manufacturing and Crystallisation, c/o Strathclyde Institute of Pharmacy and Biomedical Sciences, University of Strathclyde, Technology and Innovation Centre, Glasgow/UK
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- P 3.36 **Exploring laser induced thermocavitation for primary nucleation control**
N. Nagalingam¹; D. Irimia¹; R. Hartkamp¹; J. Padding¹; H. Eral¹; ¹ Delft University of Technology, Delft/NL
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- P 3.37 **Modelling of Turbulent Precipitation in a T-mixer with a Coupled DNS-PBE Approach**
H. Tang¹; S. Rigopoulos¹; G. Papadakis¹; ¹ Imperial College London/UK
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- P 3.38 **Tuning Interface Interactions to Facilitate Heterogeneous Nucleation**
D. McKechnie¹; P. Mulheran¹; J. Sefcik¹; K. Johnston¹; ¹ University of Strathclyde, Glasgow/UK
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- P 3.39 **The role of pre-nucleation clusters in the crystallization of gold nanoparticles**
R. Ramamoorthy¹; E. Yildirim²; P. Roblin¹; L. Lacroix²; I. Rodriguez-Ruiz¹; G. Viau²; S. Teychené¹; ¹ INP - ENSIACET - Ecole Nationale Supérieure des Ingénieurs en Arts Chimiques Et Technologiques, Toulouse/F; ² INSA Toulouse, Toulouse/F
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- P 3.40 **Unveiling the importance of solution structure on the nucleation and the final morphology of gold nanoparticles by using an ultra-fast micro-mixer in coupling with SAXS**
R. Ramamoorthy¹; E. Yildirim²; P. Roblin¹; L. Lacroix²; I. Rodriguez-Ruiz¹; A. Diaz³; G. Viau²; S. Teychené¹; ¹ INP - ENSIACET - Ecole Nationale Supérieure des Ingénieurs en Arts Chimiques Et Technologiques, Toulouse/F; ² INSA Toulouse, Toulouse/F; ³ Paul Scherrer Institute, Villigen/CH
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- P 3.41 **Towards a rigorous representation of API crystallization kinetics for enabling advanced analysis and comparison**
G. Lunardon Quillo¹; S. Bhonsale²; B. Gielen¹; J. Van Impe²; A. Collas¹; C. Xiouras¹; ¹ Janssen Research & Development, Beerse/B; ² KU Leuven, Ghent/B
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- P 3.42 **Detection of concentration enhancements at nanoscale interfaces**
R. Mackay¹; D. McKechnie¹; K. Johnston²; K. Lau³; J. Sefcik¹; ¹ EPSRC Centre for Innovative Manufacturing in Continuous Manufacturing and Crystallisation, c/o Department of Chemical and Process Engineering, University of Strathclyde, Glasgow/UK; ² Department of Chemical and Process Engineering, University of Strathclyde, Glasgow/UK; ³ University of Strathclyde, Glasgow/UK
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- P 3.43 **On the possible stereoselectivity of Non-Photochemical Laser Induced Nucleation**
M. Briard¹; C. Brandel¹; V. Dupray¹; G. Coquerel¹; ¹ Normandie Université, Rouen/F
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- P 3.44 **Solubility and Nucleation Kinetics of a Homologous Series of 8 Representative Diesel n-Alkanes (C₁₆ – C₂₃) in Toluene & Dodecane**
A. Jackson¹; K. Roberts¹; R. Downie²; P. Dowding²; ¹ University of Leeds, Leeds/UK; ² Infineum UK Ltd., Abingdon/UK
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- P 3.45 **Predicting temperature dependent solubility from thermodynamic data measured at a single temperature: Application to glycine polymorphs**
A. Manson¹; L. Lue¹; J. Sefcik¹; ¹ University of Strathclyde, Glasgow/UK
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- P 3.46 **Determining the solubility of Y₂(SO₄)₃ in H₂O-C_nH_{2n+1}OH systems for the recovery of rare earth elements using antisolvent crystallization.**
J. Du Plessis¹; J. Chivavava¹; A. Lewis¹; ¹ University of Cape Town, Cape Town/ZA
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- P 3.47 **Modeling kinetics of secondary nucleation facilitated by inter-particle energies**
B. Ahn¹; L. Bosetti¹; M. Mazzotti¹; ¹ ETH Zurich/CH

P 3.48 **Predicting relative solubilities with molecular dynamics simulations**
Z. Bjelobrk¹; D. Mendels²; T. Karmakar³; M. Parrinello³; M. Mazzotti¹; ¹ ETH Zurich/CH; ² University of Chicago, Illinois/USA; ³ Istituto Italiano di Tecnologia, Genova/I

P 3.49 **Insights into Intermolecular Interactions of Spironolactone Solvates**
L. Jia¹; L. Zhou²; Q. Yin²; ¹ Tianjin University, Tianjin/CN

POSTER SESSION III

Crystallization & Precipitation in Fine Chemical, Specialty & Life-Science Industries

Posters will be discussed on Wednesday, 1 September 2021, 10:30 – 12:00

P 4.01 **Difference in particle morphology of betamethasone by the addition of bio-surfactant between spray-drying and freeze-drying**
K. Kadota¹; H. Uchiyama¹; Y. Tozuka¹; ¹ Osaka University of Pharmaceutical Sciences, Osaka/J

P 4.02 **Solid phases relations and thermal deformations of L-serine and L-alanine**
R. Sadovnichii¹; L. Kryuchkova¹; E. Kotelnikova¹; H. Lorenz²; ¹ St. Petersburg State University, St. Petersburg/RUS; ² Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg/D

P 4.03 **The Continuous Operation of Parallel Placed Tubular Micro-Nucleators**
B. Rimez¹; ¹ Secoya technologies, Louvain-la-Neuve/B

P 4.05 **On the Similitude of Technical Precipitation**
H. Rehage¹; J. Orthey¹; M. Kind¹; ¹ Karlsruhe Institute of Technology (KIT), Karlsruhe/D

P 4.06 **Digital Design of crystallization: Impact of particle size & shape measurement on predictive capacity of calibrated mechanistic models**
J. Webb¹; N. Mitchell²; R. Taylor³; K. Foster²; S. Ward-Smith³; P. Kippax³; ¹ Syngenta, Bracknell/UK; ² PSE - A Siemens Business, London/UK; ³ Malvern Panalytical Ltd., Malvern/UK

P 4.07 **Preparation of mesoporous calcium carbonate by crystallization processing**
S. Yamanaka¹; K. Sridhar¹; K. Kadota²; H. Uchiyama²; Y. Tozuka²; Y. Yusof³; ¹ Muroran Institute of Technology, Muroran/J; ² Osaka University of Pharmaceutical Sciences, Takatsuki/J; ³ Universiti Putra Malaysia, Selangor/MAL

P 4.08 **Achieving particle size and impurity control for a continuous crystallization and wet milling process using a digital design approach**
N. Mitchell¹; C. Burcham²; F. Calado¹; S. Myers²; S. Pereira¹; ¹ PSE - A Siemens Business, London/UK; ² Eli Lilly and Company, Indianapolis/USA

P 4.09 **pH-sensitive polymethacrylate derivatives Eudragit E100 & L100 nanoparticles preparation in aqueous medium**
 F. Ofridam¹; N. Lebaz¹; E. Gagnière¹; D. Mangin¹; A. Elaissari²; ¹ University Claude Bernard Lyon-1/ CNRS, LAGEPP-UMR 5007, Villeurbanne/F; ² University Claude Bernard Lyon-1/ CNRS, ISA-UMR 5280, Villeurbanne/F

P 4.10 **Towards enhanced understanding of sono-crystallization for pharmaceuticals**
D. Pohlman¹; M. Boukerche²; H. Shariff³; N. Nere⁴; ¹ Abbvie, North Chicago/USA; ² Process Research And Development/AbbVie Inc., Chicago/USA; ³ Missouri University of Science and Technology, Rolla, MO/USA; ⁴ AbbVie Inc., North Chicago/USA

P 4.11 **Extending the scope of impedance spectroscopy as a PAT-tool during crystallization**
 C. Eder¹; H. Briesen¹; ¹ Technical University of Munich, Freising/D

P 4.12 **Using solvent additives in melt crystallization of high-viscous organic mixtures**
M. Ila¹; M. Louhi-Kultanen¹; E. Temmel²; M. Stepanski³; J. Singh⁴; B. Gevers Deynoot⁴; E. de Jong⁴; ¹ Aalto University, Espoo/FIN; ² Sulzer Chemtech Ltd., Allschwil/CH; ³ Sulzer Chemtech Ltd., Winterthur/CH; ⁴ Avantium, Amsterdam/NL

P 4.13 **Understanding the relationship between the crystal structure of different solid forms of quercetin and their physical properties using syntonomic modelling**
P. Klitou¹; I. Rosbottom¹; E. Simone¹; ¹ University of Leeds/UK

P 4.14 **Experimental characterisation and population balance modelling of batch cooling crystallisation of hexamine in ethanol**
R. Leeming¹; T. Mahmud¹; K. Roberts¹; E. Simone¹; N. George²; ¹ University of Leeds/UK; ² Syngenta, Bracknell/UK

- P 4.15 **Comparison of Isolation-Free Continuous Crystallization Operations: Falling Film Solution Layer Crystallization and Confined Suspension Crystallization**
R. Lopez-Rodriguez¹; M. Harding¹; G. Gibson²; K. Girard³; S. Ferguson¹; ¹ University College Dublin, Dublin/IRL; ² Pfizer Limited, Cork/IRL; ³ Pfizer Inc. Worldwide Research and Development, Groton/USA
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- P 4.16 **Analysis of the Crystallisation Behaviour of the Diastereomer System of DL-arabinose and DL-xylose**
B. Tyson¹; C. Pask¹; N. George²; E. Simone¹; ¹ University of Leeds/UK; ² Syngenta, Jealotts Hill/UK
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- P 4.17 **Separation strategies for valorization of lignin by targeted molecular weight fractionation**
A. Ponnudurai¹; P. Schulze¹; A. Seidel-Morgenstern²; H. Lorenz¹; ¹ Max Planck Institut für Dynamik komplexer technischer Systeme, Magdeburg/D; ² Max Planck Institut für Dynamik komplexer technischer Systeme / Otto-von-Guericke Universität Magdeburg/D
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- P 4.18 **Digital design of a robust continuous crystallization process: Using mechanistic modelling tools to minimize material requirements at the R&D stage**
B. Mehta¹; C. Brown²; N. Mitchell¹; B. Williams¹; ¹ PSE - A Siemens Business, London/UK; ² University of Strathclyde, Glasgow/UK
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- P 4.19 **Reactive crystallization kinetics of K₂SO₄ from picromerite-based MgSO₄ and KCl**
A. Albis¹; H. Lorenz²; Y. Jiménez³; T. Graber³; ¹ Universidad de Antofagasta/RCH; ² Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg/D; ³ Universidad de Antofagasta/RCH
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- P 4.20 **Sonochemical Synthesis of Double Salt Compound**
S. Kamei¹; M. Matsumoto²; S. Furukawa¹; ¹ Nihon University, Izumi-cho, Narashino, Chiba/J; ² Nihon University, Shinnei, Narashino, Chiba/J
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- P 4.21 **Continuous chiral resolution by diastereomeric salt formation of racemic Ibuprofen in a Couette-Taylor crystallizer**
L. Marc¹; J. Schneider²; G. Coquerel¹; ¹ Université de Rouen Normandie, Mont-Saint-Aignan/F; ² Seqens, Porcheville/F
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- P 4.22 **Thermal deformations of the crystal structures of L-aspartic, DL-aspartic and β-L-glutamic amino acids**
R. Sadovnichij¹; H. Lorenz²; E. Kotelnikova¹; ¹ Sant Petersburg State University, Saint Petersburg/RUS; ² Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg/D
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- P 4.23 **Crystallization-based Purification of Multicomponent Plant Extracts: The Case Study of Artemisinin**
S. Wünsche¹; S. Triemer¹; G. Vu¹; A. Seidel-Morgenstern²; H. Lorenz¹; ¹ Max-Planck-Institut für Dynamik komplexer technischer Systeme, Magdeburg/D; ² Max-Planck-Institut für Dynamik komplexer technischer Systeme & Otto-von-Guericke-Universität, Magdeburg/D
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- P 4.24 **Control of impurity profile and crystal morphology through crystallisation process design**
A. Jawor-Baczynska¹; L. Agnew¹; G. Howell¹; N. Adlington¹; ¹ AstraZeneca Macclesfield, Macclesfield/UK
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- P 4.25 **Characterization of a Small-Scale Crystallizer using Multiphase CFD Simulations and X-Ray Tomography Measurements**
R. Achermann¹; R. Adams¹; H. Prasser¹; M. Mazzotti¹; ¹ ETH Zurich/CH
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- P 4.26 **A Selective Dissolution Process Featuring a Hydrocyclone for the Removal of Fines in Crystallization**
P. Binel¹; M. Mazzotti¹; ¹ ETH Zurich/CH
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- P 4.27 **Seeded batch protein crystallization in a meso oscillatory flow reactor**
F. Castro¹; A. Ferreira¹; J. Teixeira²; F. Rocha¹; ¹ Faculty of Engineering - University of Porto/P; ² University of Minho, Braga/P
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- P 4.29 **A Contribution to the Melt Phase Diagram and Solid-State Forms of Chiral Drug Aminoglutethimide**
B. Saikia¹; F. Cascella²; A. Seidel-Morgenstern¹; H. Lorenz¹; ¹ Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg/D
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- P 4.30 **Beyond Structure Determination: Crystallisation as a Purification Unit Process for Proteins and Peptides**
 I. Rosbottom¹; F. Link¹; W. Chen¹; N. Mitchell²; J. Heng¹; ¹ Imperial College London, London/UK; ² PSE - A Siemens Business, London/UK
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- P 4.31 **Insights on the formation and dissociation mechanisms of cyclopentane hydrate obtained by using calorimetry and optical microscopy**
R. Ramamoorthy¹; J. Torrè¹; I. Rodriguez-Ruiz¹; S. Teychené¹; ¹ INP - ENSIACET - Ecole Nationale Supérieure des Ingénieurs en Arts Chimiques Et Technologiques, Toulouse/F

- P 4.32 **A novel strategy for deracemization using periodic fluctuations of supersaturation**
K. Intaraboonrod¹; A. Flood²; ¹ Vidyasirimedhi Institute of Science and Technology (VISTEC), Rayong/T; ² VISTEC, Rayong/T
- P 4.33 **Effects of crystallization conditions on the physical properties of cocoa butter – based oleofoams: a multi-technique approach**
L. Metilli¹; M. Holmes¹; M. Povey¹; A. Lazidis²; S. Marty-Terrade²; J. Ray³; E. Simone¹; ¹ University of Leeds/UK; ² Nestlé Product Technology Centre Confectionery York, York/UK; ³ Nestlé Research Vers-chez-les-Blanc, Lausanne/CH
- P 4.34 **Flow-driven Crystallization of Lithium Phosphate in Microchannels**
M. Emmanuel¹; D. Horváth¹; Á. Tóth¹; ¹ University of Szeged/H
- P 4.35 **Investigating Moisture-Induced Crystallisation By Dynamic Vapour Sorption**
M. Naderi¹; M. Guo²; D. Burnett³; ¹ Surface Measurement Systems, London/UK; ² Surface Measurement Systems (SMS), London/UK; ³ Surface Measurement Systems (SMS), Allentown/USA

POSTER SESSION IV

Integrated Process Design: Crystallization Process Design in the Industrial Process Chain

Posters will be discussed on Thursday, 2 September 2021

10:30 – 11:30

- P 5.01 **Workflow Towards Melt Crystallization Process Design in Specialty Chemistry**
M. Lührmann¹; S. Schröder¹; L. Hohmann¹; ¹ Evonik Operations GmbH | Technology & Infrastructure, Marl/D
- P 5.03 **Precipitation of Cu/ZnO on a quasi-continuous filter belt apparatus**
S. Höving¹; B. Nierhauve¹; N. Kockmann¹; ¹ TU Dortmund University, Dortmund/D
- P 5.04 **Digital design of end-to-end manufacturing process for mefenamic acid using mechanistic modelling**
C. Brown¹; N. Mitchell²; F. Doerr¹; J. McGinty¹; M. Chong¹; M. Robertson¹; S. Ottoboni¹; W. Li³; ¹ University of Strathclyde, Glasgow/UK; ² Process Systems Enterprise, London/UK; ³ Loughborough University, Loughborough/UK
- P 5.05 **Using modelling tools to accelerate the design process of the innovative continuous Archimedes tube crystallizer**
J. Sonnenschein¹; R. Heming¹; M. Aghayarzadeh¹; O. Mierka¹; S. Turek¹; G. Schembecker¹; K. Wohlgemuth¹; ¹ TU Dortmund University, Dortmund/D
- P 5.06 **Towards Increased Product Quality Inside a Slug Flow Crystallizer**
A. Kufner¹; M. Termühlen¹; K. Wohlgemuth¹; ¹ TU Dortmund University, Dortmund/D
- P 5.07 **Designing a Continuous Taylor-Couette Crystallizer – Residence Time Distribution and Suspension Characteristics**
M. Etmanski¹; M. Breloer¹; G. Schembecker¹; K. Wohlgemuth¹; ¹ TU Dortmund University, Dortmund/D
- P 5.08 **New soft sensor design for a batch crystallization process based on solute concentration**
L. Brivadis¹; V. Andrieu¹; É. Chabanon¹; E. Gagnière¹; N. Lebaz¹; U. Serres¹; ¹ Université Lyon 1, Laboratoire d'Automatique et de Génie des Procédés, UMR 5007, CNRS—ESCPE, Villeurbanne/F
- P 5.09 **New inversion method for the multi-shape CLD-to-PSD problem with spheroid particles**
L. Brivadis¹; L. Sacchelli¹; ¹ Université Lyon 1, Laboratoire d'Automatique et de Génie des Procédés, UMR 5007, CNRS—ESCPE, Villeurbanne/F
- P 5.10 **Digital design of crystallization and Advanced Process Control using mechanistic models**
J. Mack¹; R. Parekh¹; F. Tahir¹; C. Brown²; J. Johnston²; J. Robertson²; N. Mitchell³; A. Florence²; ¹ Perceptive Engineering - an Applied Materials Company, Daresbury/UK; ² CMAC/ University of Strathclyde, Glasgow/UK; ³ PSE - A Siemens Business, London/UK
- P 5.11 **Size and Shape Engineering of Needle-like Particles: Process Development and Process Control**
A. Rajagopalan¹; S. Bötschi¹; F. Salvatori¹; P. Binel¹; M. Morari²; M. Mazzotti¹; ¹ ETH Zurich/CH; ² University of Pennsylvania, Philadelphia/USA
- P 5.12 **Process Development for Size and Shape Manipulation of plate-like crystals**
D. Biri¹; A. Jaeggi¹; P. Binel¹; A. Rajagopalan¹; M. Mazzotti¹; ¹ ETH Zurich/CH

- P 5.13 **A crystallisation development workflow for the manufacturability enhancement/improvement of active pharmaceutical ingredients**
H. Siddique¹; ¹ CMAC National Facility, Glasgow/UK
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- P 5.14 **Model-based optimal choice of pressure-driven withdrawal method from stirred suspensions**
R. Achermann¹; V. Wiedmeyer¹; M. Hosseinalipour¹; S. Güngör¹; M. Mazzotti¹; ¹ ETH Zurich/CH
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- P 5.15 **Multidimensional particle characterisation from in-situ imaging using deep learning and transfer learning**
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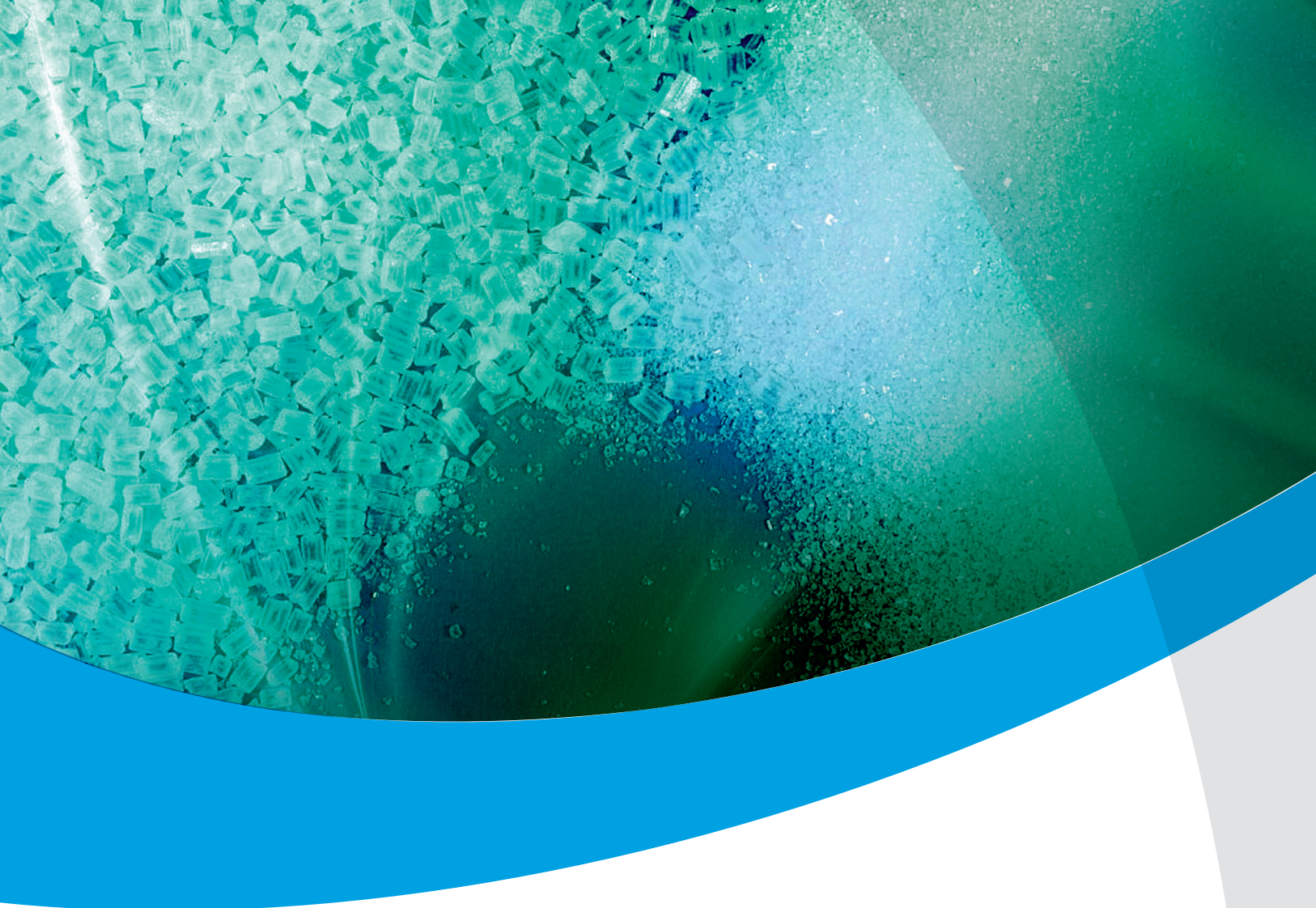
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