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Particle technology's contributions to the major challenges of the 21st century A predictive retrospective as a *particular* birthday present of IChemE

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ABSTRACT

In 2122, IChemE - Institution of Chemical Engineers – will celebrate its bicentenary. This article presents as a retrospective the years 2022–2122 and summarizes the progresses (to be) made in the field of particle technology until 2122, i.e. during the second century in the life of the yet young IChemE.

A century earlier, in 2008, the U.S. National Academy of Engineering (NAE) announced the grand challenges for engineering in the 21st century. The list has been compiled by a committee under the chair of William Perry[1] and comprises a series of challenges to which particle technology will obviously make a sound contribution, such as …

- Make **solar energy** affordable
- Provide energy from **fusion**
- Develop **carbon sequestration** methods
- Provide access to **clean water**
- Engineer better **medicines**
- Engineer the tools for scientific discovery

Particles are everywhere, be it due to natural or human activities and their formulation, production, handling and characterization has a major influence on the quality of many aspects of life.

We summarized the visions of leading scientists and practitioners in the field of particle technology (and around) in order to discover their opinions summarizing the progresses in this field (to be) made in the 21st century – and the societal impact related to these. We allowed them to *dream, to wish, to be forward-looking, to be optimistic*[2] in the framework of a bicentenary.

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[1] he has been former U.S. secretary of defense and professor of engineering at Stanford but has never written an engineering handbook

[2] Optimism, according to Merriam-Webster "a doctrine that this world is the best possible world", being probably not the predominant mindset in 2022.

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1. Introduction

The 20th century had, to put things diplomatically, a catastrophic start: Human aggression was targeting other humans leading to the death of millions. Later in the century, lessons seemed to be learned and IChemE's first century's anniversary could almost have been the contemporary witness of a better world. In this context, particle technology had, alike many other technological disciplines, benefitted from the post WW2 economic miracle years and had, based on the increased scientific interest (Heywood, 1937) of the early 20th century, evolved very rapidly from 1960 to 2000. It had then been driven by a strong academic and industrial network which focussed on theory (Rumpf, 1977), quality of measurement (Willeke and Baron, 1993), standards (Leschonski, 1986), and education (Scarlett, 2002). Important themes had been economic growth, competitiveness, progress. Its beginning, applied to engineering fields, is usually dated back to the 1960′s decade with the work of Herdon and the book "Small Particle Statistics", and later to the set-up of some research groups in the field, namely in UK at the Universities of Loughborough and Bradford, and in Germany and France at the Universities of Karlsruhe and Nancy, respectively. Another important milestone is the organization of the first Particle Size Analysis Conference in 1970, in Bradford, UK. Additionally, the journal of Powder Technology was first published in 1968. Later, in the 1970′s decade, Particle Technology started to be a topic included in several Chemical Engineering degrees. Along the 1980′s, Particle Technology applied to the Engineering field became progressively more structured, with several books being published, and establishing a multidisciplinary approach to engineering problems. In fact, it is well known that particles are present in 80% of the final or intermediate products of process industries.

The product of the efforts was the refinement of the technology, the use of standard operating procedures and the creation of a solid laboratory-based culture of particle characterization quality assurance. This was based around well tested and proven tools supported by end user and supplier-based experts whose deep knowledge was won from practical experience and theoretical advances. However, this success has led to the commoditization and segmentation of the discipline and as the older generation of experts has retired there has been a loss of the wide spread fundamental knowledge and fundamental skills.

One hundred years later, the 21st century did not get of to a good start either. A global – albeit short – economic crisis, the first really worldwide pandemic for more than a hundred years, the decades long exit of the former United Kingdom from the European Union and a major war in Europe did remove innovation from the front of any politician's mind. Furthermore, citizens and politicians slowly achieved a broader consciousness that the current resource intensive and polluting lifestyle was destroying their own habitat. Industry transformed into a resource savings machine, thus inadvertently helping with the global warming crisis. The societal impact of this transformation was unexpectedly strong - and particle technology at its forefront.

Today in 2122, alike a century earlier, nobody can understand the quarrels which span the first fifty years after the centenary of the IChemE in 2022, of humans destroying the only place they had to live.

IChemE is one of the main roots of the pan-European Chemical Engineering Society, which ensures that the contributions of the discipline are not neglected in the wider societal discourse. Engineers were on both sides of the fight whether individual mobility should remain the future of transportation and if so whether it remain based on the combustion engine and fuelled either by refined fossil oil or so-called e-fuels. Neither proved to be a viable option in a carbon emission restricted world. With the advent of the angstrom designed particles and their superior ability to store and handle electrons, smoking cars were squeezed out of the cities within a decade and off the Autobahn ten years later. Angstrom design took the technologies used for shaping minute electronic structures e.g. in computing chips, made them three dimensional and revolutionized the manufacturing of performance particles.

Particles also became the solution for one of the pressing long-term issues of the highly industrialized world. Biologically active substances have been just as much a blessing in medicine, animal health and crop protection, as they have been a problem. Much of the administered quantities do not arrive at the right place in the body (human medicine) or do not impact the plant (crop protection) and if so, they arrive at the wrong time when the organisms cannot utilize it. The residual quantities then are the cause of development of drug resistances. Particles which will remain inert if the conditions are wrong and release their payload when the respective triggers are met, have lessened this issue to a large extend. Today researchers work on the next generation of these particles, which will not only control the release of its payload but also ensure its decomposition into inert matter if it is not used.

2. The 21st century: focus on particle technology

2.1. *The place of particle technology in the 21st century*

To say particles are ubiquitous is a phrase commonly used for centuries and yet still very relevant today and will do for centuries to come. Particles can be found in a wide number of products we use every day in food to medicines, in applications for energy storage sector through to the environmental either existing naturally or produced for environmental protection. Particles range in size and dimensions from the nano and micro through to larger scales. Technologies have evolved in the making and handling of these particles and advances in characterisation techniques have enabled us to understand so much more about particles from X-rays to electron microscopy to "look" into the arrangements of atoms/molecules at the atomic length scales.

The initial developments, after the area became progressively more structured, are amazing. In general, it can be stated that in the last 50 years the strategy of the four Ms, Making and Manipulating products linked to Measuring and

Modeling, has gained progressively more and more importance in the field of Particle Technology.

The broad concept of "Particle Technology" has in the early 21st century been better perceived by the whole society, i.e. by the scientific and industrial communities, leading to a more comprehensive and structured understanding of the field of particle technology, overpassing excessive compartmentalization, favouring the development of comprehensive approaches, as well as by decision makers who discovered the relevance of particulate systems such as aerosols. Particle Technology will continue to increase its relevance in both process and product engineering, in the most diverse sectors, and will be essential and recognized as such, for the development of future products crucial for humankind.

2.2. *The focus of research works in the 21st century*

The unique properties of particles remain intriguing, from their size, size distribution, porosity, shape through to the arrangement of the molecules within their internal structure that make up the particle. In the 21st century we worked successfully on particle engineering – making and optimising the properties of particulate materials. The research focus is to understand the role of the solid interface in particle system performance - how the solid-solid, solid-liquid or solid-vapour interactions are … we argue the interface is critical as all interactions first occur at the interface. Particle scientists characterised much of the bulk properties in the 20th century, leading successfully to international standards for example for silo design. But sometimes the interfacial properties were neglected. The interfacial properties are still not very well understood… Wolfgang Pauli, was reported to say that, "God made the bulk; the surface was invented by the devil." Works have demonstrated the particles are anisotropic and heterogeneous, with a distribution of properties in a population. More recently, particles are engineered with unique pore dimensions and surface chemistry to enable controlled nucleation and crystallisation or complex organic solids such as biopharmaceuticals, such as peptides and proteins. These have remained challenging due to the difficulty to crystallise large molecules. Crystallisation has been widely used in industry for the isolation and purification of small molecule pharmaceuticals.

The surface is important… but it is not the only thing that matters. Size does matter. Shape does matter. Roughness does matter. The internal arrangement of the molecules or atoms matter. The particle properties will influence powder handling performance through to product performance. Particles are 3D and we must describe their characteristics as such and not only 1D. We need to be able to capture the diversity and range in such particle properties to be capable of describing more accurately powder behaviour. Modelling tools have advanced but critically have also become more accessible. The days where research groups only exist as a purely experimental or modelling group is limited. There is so much synergy between model/experiments across the multiple length scales in particle technology. The experimental and modelling groups collaborating together became more common.

The importance of particle technology concepts and strategies for developments in the sector of medicine and health and also in the pharmaceutical sector have progressed a lot, in order to produce new formulations, tuning them to achieve the required performance, with a strong movement towards the production of specialty products, as for instance the production of biocompatible particles and materials optimizing the particles structure, and also the production of intelligent particles. The development of these new products will be more and more often based on the use of modelling strategies for both the design of the process and for the prediction of the behaviour of the particles in the target application. The production of these intelligent/specialty particles eventually requires process miniaturization and is also a challenge for process design. Still related to these developments, it is possible, in the case of health applications, to synthetize particles directly in the human body, with an improved efficiency, producing in situ particles adapted to body conditions.

In-line with the developments mentioned above, but not only, a strong progress linked to nanotechnology is established, including, of course, an intense progress in the development of new nanoparticles and also their production and processing processes, with new technologies appearing first at the lab level and moving progressively into market and production scale, in sectors such as electronics, health and welfare, environment remediation, just to mention a few. The required stronger investment in the fields of characterization and manipulation of nanoparticles with the development of new techniques/strategies have been made.

Also, in relation to nanotechnology, but not only, particle technology assumes a strong presence in the electronics field, namely with new ways to produce miniature electronic components always more and more efficient, but mainly in the sensors area, contributing to the development of new and more sophisticated and versatile sensors for a wide variety of applications, including health and environment, which requires again the production of intelligent nanoparticles.

A very important field where Particle Technology is of much stronger relevance is the field of environment, generally speaking, with advances in this area relying necessarily on particle technology concepts. In this sector the development has been essential of more accurate or cheaper and automatic techniques to monitor the presence of particles, to assess their characteristics and, simultaneously, to develop more efficient techniques/processes to remove them, with the possibility of tuning automatically those processes to different situations/environments, which can change along time and place.

Connected to the environment applications, Particle Technology plays an essential role in climate change mitigation plans. Some possibilities are for instance in the development of biomimetic particles to absorb and release heat in intelligent buildings, mimicking what happens with plants or some microorganisms. In the sector of agriculture and related to water scarcity, particles can be used to irrigate plants in an efficient way, slowly releasing water in the roots area, substituting traditional irrigation procedures. Also related to the water scarcity problem, new particles are essential to develop new water purification and desalination technologies leading, eventually, to revolutionary technologies which could not be imagined at IChemE's first century event in 2022.

Particle Technology has contributed to the development of strategies to enable earth cooling. Imagine, for instance, the installation in the earth atmosphere of clouds of intelligent particles which will work as heat absorber points, producing also energy in an efficient way.

Another issue is particles' evaluation in production processes: particle characteristics evaluation on-line or in-situ in industrial processes are a requisite, in order to allow a more effective control of the process and of the final products. In this field, tomographic and imaging techniques, using different approaches, went on evolving and became more accurate, mapping, instantaneously, what is the situation in the process equipment of the particulate phase (characteristics, distribution, etc.). Artificial intelligence and machine learning applied to particle technology will play an important role in this field. Still in the area of on-line measurements the development of hybrid techniques, allowing the simultaneous evaluation of different particle properties, is a reality in 2122.

3D printing is another area where Particle Technology played an essential role. Whilst in 2022 the majority of European households were only equipped with 2D (paper) printers, almost none lacks of a 3D printer in 2122. This is also a field of new importance in different sectors, such as sensors and electronics, automotive industry, miniaturized processes, among others. A detailed knowledge of the behaviour of particles in those new fabrication processes is critical for their optimization and to expand their application to a wider range of sectors.

In the field of particle characterization, strong developments were possible with a continuous and sometimes disruptive evolution of particle characterization techniques. One of the areas that faced a strong development is the progressive movement to multi-property measuring techniques, combining, in the same equipment, the possibility of assessing different properties of the particles (size, shape, composition, etc.), and also monitoring their evolution with time. Also in this field, radiation scattering techniques which are rather friendly and well installed at both research and quality control levels, are no more restricted to light scattering, and will progressively evolve to their use in more realistic characterization conditions, important at the industrial level, especially allowing the characterization of more concentrated samples, in an accurate way, which required the improvement of signal acquisition sensors and also of the data treatment models. Also, in order to enable more realistic particles characterization, it is no longer necessary to consider the particles as pseudo-spherical, as the models applied in signal deconvolution procedures became more detailed and realistic. Artificial intelligence plays a stronger role in the field of particles characterization, in order to allow achieving the objectives mentioned above.

The recent commercialization of customized multi-functional equipment, combining in the same equipment different techniques (e.g. for size and shape analysis, structure analysis, composition, etc.), which can be selected and blended by the user depending on the target and needs of the characterization, allowing the tuned and customized evaluation of different properties of the particles are of outmost importance in industry.

Virtual measurements and virtual laboratories, as already mentioned by Trichard in 1999 are now a reality, enabling remote services and contributing to a wider and easier dissemination of particle characterization methods, including in remote areas, which are of particular relevance in the case of environmental applications.

The development of flexible and predictive models allows a more accurate and easy design of process equipment handling particles, providing an easy way to adjust the process to the production of the required particles/products. Particle centred models, namely population-based models, are now the main relevant ones in this area. A movement from single property models to multi-property models occurred, allowing a more detailed description of the particles. The more efficient solution of progressively more complex models requires the use of efficient data handling strategies, enables more efficient and accurate model solution procedures, and, most certainly the coupling with artificial intelligence.

3. Case studies - progresses made in the 21st century

3.1. *Case study 'crystallization'*

Indeed, the world we live in today is -compared to 2022- a better place, also thanks to crystallization. Most of the objectives set up by crystallization scientists and engineers one century ago were eventually met. Crystallization contributed to the ambitious goal of halving greenhouse gases emissions every decade since 2022, resulting in a global warming of "only" 1.5 °C by 2100. Crystallization has contributed to this goal as it played (and still plays) a crucial role in the battery industry. Batteries are, in fact, necessary to deal with the intermittent nature of renewable energy sources, which empower today's world. Reactive crystallization, in particular, is a key step in producing many battery materials and fractional crystallization is employed in battery recycling. This latter allows to separate the different metals involved in the production of battery materials (cathodes in particular). Crystallization is also involved in the extraction of critical raw materials from the sea, following the circular economy concept. The Mediterranean Sea is now an open mine, that through its salt works provide us, not only with table salt, but also, thanks to crystallization, with magnesium, lithium and energy. The energy is instead produced by employing reversed dialysis and by making use of osmotic power in general.

Improvements in process modelling and control have made it possible to reduce energy consumption in crystallization processes, contributing to saving the amount of energy that resulted in reduced emissions.

Crystallization has also played a crucial role in fighting diseases caused by antibiotic resistant bacteria and new viruses resulting from zoonoses. The pharmaceutical industry has been, in fact, profoundly transformed by the advances in crystallization. Solvent screening and the identification of optimal operating conditions have become much faster, thanks to robotic laboratory automation and artificial intelligence, which are now omnipresent in crystallization laboratories. As already mentioned, process control, that allows to produce the powders with the ideal characteristics, has been revolutionized by the development of innovative probes and monitoring tools, which now allow to measure, just to cite one example, not only one crystal size (in one dimension), but also crystal morphology (in two and three dimensions). These powerful online monitoring tools, coupled with surrogate models, built on machine learning tools, have made it possible for crystallization processes to be controlled on-the-fly with unprecedented accuracy. This has resulted in faster time-to-market and seamless scale-up, from the laboratory to the industrial scale. Research in crystallization and precipitation has also played an important role in the production of mRNA vaccines, where solvent-displacement is often used to create supersaturation and drive the formation of lipid nanoparticles, where the mRNA molecules are encapsulated. The pharmaceutical industry has also benefited from important advancements in the field of enantiomer separation via preferential crystallization.

Crystallization has been revolutionized also with new and innovative ways for controlling nucleation, which is in nature a stochastic phenomenon, by employing for example laser light and ultrasounds.

Research in crystallization, on the theory of nucleation, has helped in understanding many natural phenomena, such as ice crystal formation and rain drops generation in clouds, helping us in mitigating the effect of climate change.

At last, it is important to mention that the use of multiscale modelling, combining quantum chemistry calculations, molecular dynamics (full-atom and coarse grained), population balances and computational fluid dynamics, has resulted in the development of high-fidelity computational tools, which require limited experimental activity for their validation. This has impacted crystallization transversally, providing crystallization scientists and engineers with tools that can be employed during process development, design and optimization. Thanks to these advancements, it is finally now possible to design a crystal and to identify the ideal process that can be used to produce it without the trial and error procedure employed in the past.

3.2. *Case study 'aerosol technology'*

Aerosol technology is in 2122 ubiquitous. What had been called cleaner air in 2022, now is called even in non-scientific papers: cleaner aerosol. The fluid (air) plus particles, gases and droplets are considered now as one system: "The aerosol". This started right after the COVID-19 pandemic once recognized and communicated to the general public what aerosols are and that aerosols play an important role in transmitting the disease.

Nowadays, the aerosol quality level is visible everywhere and stays within healthy limits. The foundation of a scientific setting of health levels started about 100 years ago. It gained momentum with the EU HORIZON EUROPE call on indoor air quality and health. Innovation research actions like LEARN provided the scientific database and evaluation for setting the right aerosol levels in schools, fostering healthy and optimal conditions for learning. A cognitive study was included as well as optimization of filtration to achieve and control the aerosol level incl. VOC and ultra-fine particles. Nowadays pupils and students are at least one grade better than 100 years ago. Monitoring these aerosol levels gained also momentum. Nowadays, sensors are almost everywhere. What has been the GPS in cellular phones 100 years ago, is now ultra-fine particle sensors in almost every device, special textiles, or other smart materials.

Advances in particle technology have made it possible to not only measure from nano- to micro-scale particle size and electric charge at low cost, but to distinguish shape and chemical composition of particles and droplets. In addition, advances in gas molecule characterization have made it possible to distinguish between harmful and healthy gases. In combination with AI and machine learning, now the aerosol level is calculated in real-time and predictions are more accurate than weather forecasts have been 100 years ago. This enabled visualization of aerosol quality levels. This strengthens the demand for cleaner aerosols, former cleaner air, and led to innovations in filtration technology.

Filtration technology has advanced in many ways. The design of filter media as well as of filtration devices is done now fully virtual. It starts with the melt chemistry and does not stop at the 3D printing of the fibrous structure. The shape of each individual fibre of a filter medium is locally optimized. This started with first academic studies 100 years ago investigating topology optimization of fibres. The fibre structure is adaptive, i.e., open, or dense, depending on the filtration demand, or adaptive to better remove particles. First academic studies started 100 years ago.

For most of the filter material a circular economy has been established. Particle technology made this possible, by energy efficient separation of collected particles/droplets from fibre material. In other cases, bio-degradable material is used for filters, fibres as well as e.g., sealing. With a cradle-to-cradle approach it turned out that some used filters are a preferred input for making other materials, as additive for cleaner and more efficient incineration or other way of material processing are applied. Both topology optimization and adaptive filter media resulted in nowadays a factor 4 lower energy consumption at same efficiency level over lifetime of a filter.

Separating the useful from the harmful, has been one of the most important tasks in the last century. This comprised not only particle filtration but molecular filtration, too. The demand for cleaner aerosols and the visualization of aerosol levels, created new business like additional mobile air purifiers, upgrading HVAC systems, etc. Even a new focus on health risks like non-exhaust emissions of electric vehicles like brake, tire emissions and road abrasion needed filtration at the source or in the contaminated environment as a remedy solution. Special filtration devices, as used for the first time about 100 years ago at the fine dust hot spot Neckar Tor at Stuttgart, have now been implement along highways, crossings etc. These filtration devices contribute to more social equality and reduce environmental injustice as they improve the aerosol quality in these hot spot areas. Other steps initiated for cleaner urban aerosols are now a standard e.g. with filtration devices in subway stations.

Last not least, there are much more filtration solutions nowadays than 100 years ago, as separating the useful proved to be the key enabler for improvements or disruptive innovations. Hence, despite the transition from filtration for internal combustion engines to filtration for e-mobility, the last 100 years have been the golden age of filtration driven by digitalization, visualization and monitoring of aerosols. As there will always be a need for cleaner aerosols, former cleaner air, innovations and progress in aerosol and particle technology will continue and be needed for a healthy world.

3.3. *Case study 'A gaseous future'*

Yet at IChemE's first centenary, we were aware of the challenges of a growing population, growing worries about climate change and limited resources. Many problems can be eased by simple small bubbles. "Fine Bubble Technology" covers the generation, characterization and applications of suspensions of millions of small bubbles. They were formerly called nanobubbles but they fail the EU nano definition as they don't always have > 50% sub 100 nm nor are solid, so the correct ISO parlance is Ultra Fine bubbles.

The usages of nanobubbles are wide, but they are particularly focused on environmental applications. The bubbles are extremely surface active and highly charged so have found usage in; chemical free cleaning of road salt builds up on ironwork such as bridges (which causes corrosion) toilets, fabrics, machined parts and vegetables, seed germination (faster and helps imperfect seed germinate), plant growth (larger plants) and aquaculture (such as shrimps, larger and higher survival rates).

Environmental clean-up (oxygenation of stagnant water sources), Removal of harmful bacteria, Potential drug delivery applications of coated bubbles which can permeate into tumours more effectively than coated solid or liquid particles.

Standardisation of equipment and methods in this developing area have successfully be encouraged. Many of the technologies key benefits map on to the United Nations Sustainable Development Goals, and there have been many successful horticultural and aquaculture trials of the technology to date.

The bubbles themselves are resilient, they can last for many months unless frozen or undergoing pressure changes such as flying.

There is a great deal of interest all over the world in this technology, and a steady feed of new applications are being developed which points to a bright future for this area where a great deal can be achieved with something as simple as gas in a liquid.

4. Outlook and conclusion - The third century of IchemE

The physics of particle interactions are one of the fields where particle technology remains a challenge in the 22nd century. Even on modern quantum computers, the challenges have not lessened compared to a hundred years ago. Multibody dynamics on modern computers can handle unprecedented numbers of particles which are tracked individually. However, the laws of interaction have not been understood much better than in the early 21st century and certainly not been formulated in a way that they can be computed easily. The rapid advancement of computing power has prevented the necessary focus on efficient algorithms and suitable physical models which are needed to make a quantum leap with a quantum computer simulation.

We are currently faced with global challenges to address climate change to food security. Scientists and engineers work on the discovery of new materials, engineering novel manufacturing processes, inventing advanced characterisation and modelling tools, and many more – We believe that there has not been a better time to be a particle technologist.

Happy Birthday IChemE.

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Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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