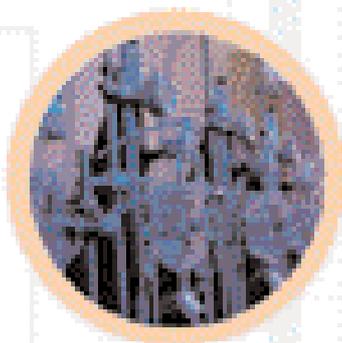
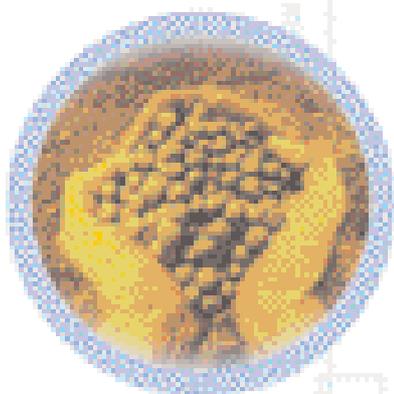


# IMPACT Faraday Partnership

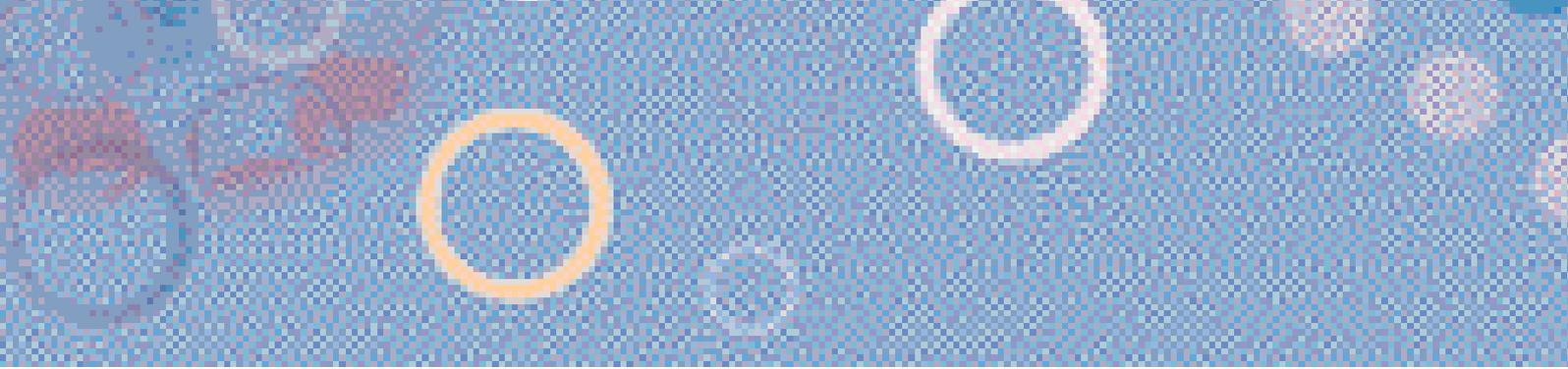
A Technology Road Map for Colloid  
and Interface Science in the UK





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# EXECUTIVE SUMMARY

Colloid science and its related technologies underpin much of the UK chemical industry including: paints and coatings; agrochemicals; pharmaceuticals; personal care; healthcare; soaps and detergents; petrochemicals; speciality and effect chemicals; and foodstuffs.

The focus of IMPACT Faraday Partnership is to support the design and development of innovative materials, and the development of new formulated products.

This report is the culmination of a consultation process with both industry and academia to identify strategic research activity in the area of colloid and interface science. The research identified is fundamental in nature, but has its origins in underpinning technological capabilities relevant to future technological needs of industry.

The report has been constructed through the logical sequencing of developing a science and technology landscape, formulating a technology road map framework, and then extracting a strategic research agenda. It is envisaged that this document will be dynamic, and will be regularly updated to reflect changes in technological needs and recognition of gained knowledge capability.

The information used in the report has been gathered through visits made to organisations by the Technology Translator team of IMPACT, and the use of two innovative brainstorming sessions. The first of these sessions was an open invitation to industry and academia, and involved close to 60 people, while the second session was a more focused event involving a mixture of 10 industrialists and academics.

Further added-value has been gained by IMPACT during this process through the identification of technology transfer opportunities across sectors, and training/learning needs of industry.

The exercise has had a strong emphasis on the priority requirements of industry, and has concentrated on the differing needs in the process of turning ingredients into manufactured products that will be of value to the customer.

Five dominant research themes were identified:

- Prediction modelling
- Controlled colloid architecture
- Controlled and triggered release
- Measurement
- Biological systems

Furthermore, detail within these themes has identified opportunities to link into other existing initiatives, synergies with other Faraday Partnerships and subsequent potential for collaboration.

It is recommended that this report is widely disseminated to the industrial and academic colloid and interface science community to elicit feedback. The objective being to obtain an agreed strategy for IMPACT Faraday Partnership, which will provide:

- A focus for IMPACT research activities
- Comparisons with Europe, the USA and Japan
- Design of future Technology/Knowledge brokering events
- Sector specific technology audits and road maps
- Development of relationships across the EU.

# 1. OBJECTIVES

The information generated in this report has been gathered following a consultation process with both industry and academia. The aim of the report is to identify strategic research activities in the area of colloid and interface science where, together, industry and academia can make a difference by providing innovative products and processes. The report will be widely distributed in order to encourage discussion between the industrial and academic communities to further refine the strategy with the intention of generating focused collaborations. Support for this collaborative research will be sought from the UK Government and the EU.

# 2. METHODOLOGY

## 2.1 Introduction

Colloid and interface science, as applied to the design, manufacture and performance optimisation of products, are universal in their effect in the following sectors: paints and coatings; agrochemicals; pharmaceuticals; personal care; healthcare; soaps and detergents; petrochemicals; speciality and effect chemicals; and foodstuffs.

IMPACT (Innovative Materials development and Product formulation by the Application of Colloid Technology) covers those aspects of industrial RD&T (Research, Development and Technology) and manufacturing that typically involve processing of some "ingredient" base into a functional product comprising a complex physical form.

A consultation process with both industry and academia to identify strategic research activity in the area of colloid and interface science has been carried out through visits made to organisations by the Technology Translator team of IMPACT, and the use of two innovative brainstorming sessions. The first of these sessions was an open invitation to industry and academia, and involved close to 60 people, while the second session was a more focused event

involving a mixture of 10 industrialists and academics. The research identified is fundamental in nature, but has its origins in underpinning technological capabilities relevant to future technological needs of industry.

## 2.2 Landscape

The report has been constructed through the logical sequencing of developing a science and technology landscape, formulating a technology road map framework, and then extracting a strategic research agenda. It is envisaged that this document will be dynamic, and will be regularly updated to reflect changes in technological needs and recognition of gained knowledge capability. A description of the science and technology "landscape" which deals comprehensively with opportunities across this vast range of commercial activity runs the risk of becoming far too general.

However, the outline landscape below steers a path between these extremes by constructing a framework in which formulation is likely to have a substantial influence on the success and competitiveness of industry in different parts of the RD&T and manufacturing chain. Common themes are highlighted where step-changes in research capability in science, engineering and technology (SET) will produce benefits across a number of different industries.

Analysis of the needs of industry suggests it is useful to summarise these within a structure described in the schematic diagram shown in Figure 1. This is one way to differentiate between stages and activities that go into the process of turning ingredients into products in order to clarify:

- where the FORMULATION of products is critical to industry
- how new research will support industrial needs by influencing formulation capability.

While this structure describes the landscape, the technology road map is the framework of future directions and opportunities which can be imposed over the landscape to identify key routes for future development.

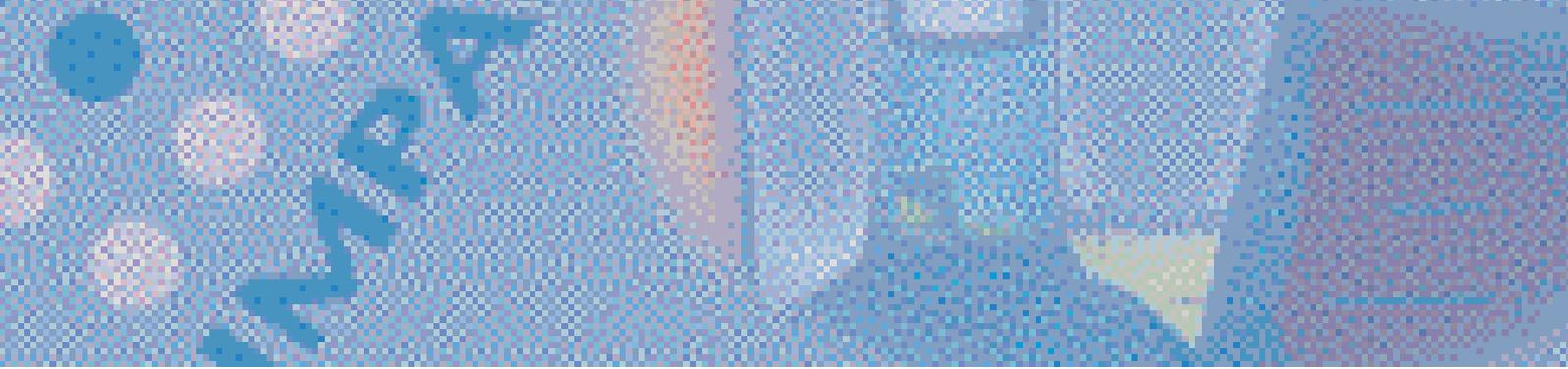
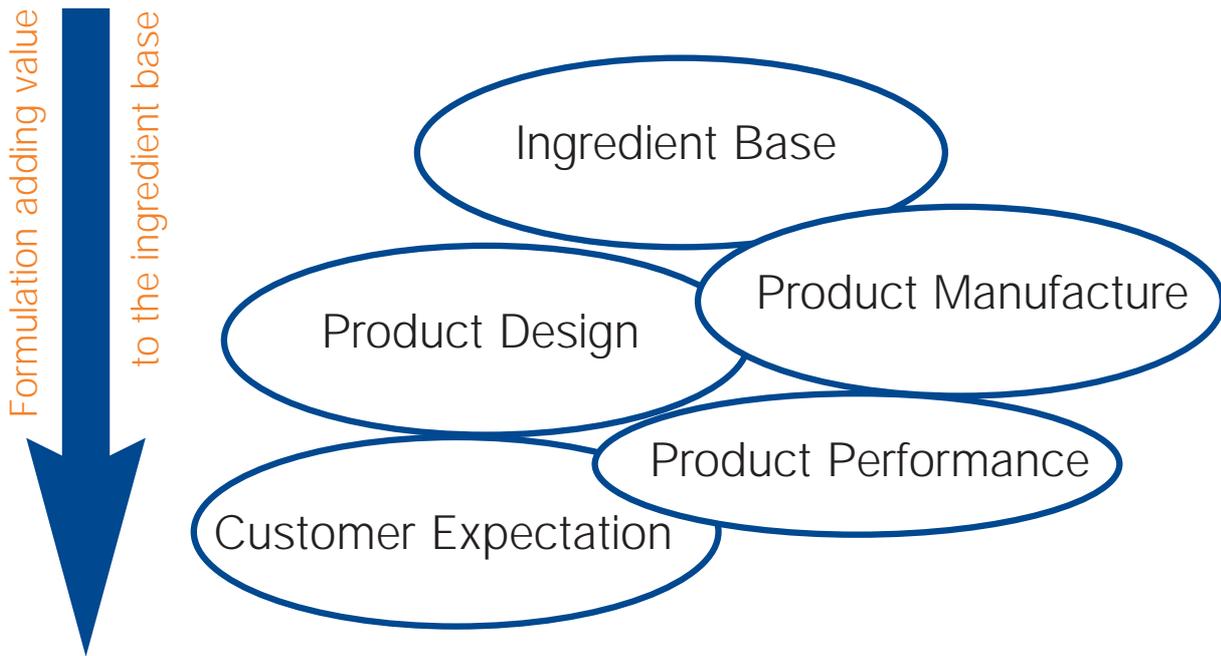


Figure 1: Generic stages of an industrial activity where colloid and formulation science are used to add value to products



### Definition of terms

**INGREDIENT BASE** – how ingredients can be manipulated (e.g. nanoparticle formation) or chosen (e.g. prediction of surfactant interactions) to optimise formulation process and product performance;

**PRODUCT DESIGN** – how to manipulate product form to deliver product performance, for example, the correlation between bulk property and microstructure;

**PRODUCT MANUFACTURE** – improving the understanding of the influence of colloid and interface science in the processing of the product;

**PRODUCT PERFORMANCE** – delivering an effect, such as, product stability, application efficacy, and mode of action of formulated product (as opposed to mode of action of active ingredient);

**CUSTOMER EXPECTATION** – research on how to formulate specifically to meet market/customer need. This is related to product design/performance, but focuses on the critical additional properties of the product over and above its primary “functional” capability, as, for example, in sensory qualities (food/cosmetics/personal care) or societal drivers (environmental concerns).



Sitting along these “routes” are the technical challenges which need to be met to allow this future to be realised, and therefore identify the key areas where research activity is most needed and/or has greatest promise of delivering step-change capability. These stages of the RD&T chain are common across nearly all of the industry sectors discussed here, but allow for some degree of focus within each to determine if there are key new capabilities that could significantly improve industrial competitiveness. Within each of the areas identified, we have undertaken an

analysis of industrial needs across a range of industrial sectors. These are shown in Figure 2. The table shows the range of industrial sectors in which colloid and formulation science plays a role in product design, performance and manufacture. The relative importance of this competency to the industry is indicated in the first line of the table (High, Medium or Low). Entries marked with an (X) indicate where the industrial needs are important factors to these industrial sectors.

Figure 2: Industry sector needs

Importance of colloid technology		High	Medium	Low	Industrial Sectors																				
High/Medium/Low		M	M	M	H	H	L	H	M	H	H	H	L	H	M	H	H	M	L	L	H				
		Aerospace	Agriculture	Automotive	Building and Construction	Chemical and Pharmaceuticals	Chemicals	Domestic Appliances	Electronics/Electrical Goods	Environmental/Plastic	Energy	Food and Drink Processing	Healthcare	Instrumentation	IT and Computing	Marine/Oil/Gas	Metals	Of and Gas	Packaging	Plastics	Power Generation	Telecommunications	Textiles		
Ingredient base	Easy/reliable Ingredient substitution		X	X	X	X	X	X		X		X	X		X	X		X	X		X	X		X	
	Components' physical form	X	X	X	X	X	X	X	X					X		X	X		X	X		X	X		X
	Product robustness (storage, manufacture, performance)		X				X				X	X	X	X		X			X	X					X
Manufacturing	Process robustness and flexibility	X	X		X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
	Smart assembly of multicomponent products	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
	Distributed facilities	X		X		X	X	X	X	X	X	X	X	X		X		X	X	X		X	X		X
	Process efficiency	X			X	X	X	X	X	X	X	X	X			X		X	X						X
Product design	Predictable product stability	X	X			X	X	X	X	X	X	X								X	X				X
	Link to manufacturing process and product performance	X	X			X	X	X	X	X	X	X			X	X		X	X		X	X			X
	More efficient products	X	X	X		X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
	Microparticle design	X	X	X		X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
	Controlled 3D architecture	X	X	X		X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
Design link to product application process	X				X						X	X												X	
Product performance	Predictable performance criteria	X	X			X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
	Performance robustness	X	X			X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
	Smart effects	X				X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
	Low environmental impact	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
Biocompatibility or bioavailability	X				X					X	X	X													
Customer expectation	User safety	X		X		X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
	Low environmental impact	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
	High performance/cost ratio			X		X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
	Personalised products					X	X					X	X	X	X	X	X	X	X	X	X	X	X	X	X
	Understand customer-product interactions					X	X					X	X	X					X						X

## 3. TECHNOLOGY ROAD MAPPING

In each of the five following sections: “ingredient base”; “manufacturing”; product design”, product performance” and “customer expectation”, the issues which industry perceive as being key strategic drivers to the future sustainability of their business are distilled into some common headings which should apply to most industry sectors.

These were used to capture, from leading experts and key innovators in the field, the current state of the art and ideas about where future directions could most productively be targeted to yield step-change benefits to meet these future needs. The state of the art expertise has been captured elsewhere and will be published in another format. This is key to identifying areas where technology transfer, from expert users in either academia or industry, can provide benefits across a greater range of UK industry.

In the subsequent sections of this document the challenging and “difficult” science is captured, where creative and radical approaches in focused collaborative research is likely to yield the greatest competitive advantage to industries, and UK SET colloid and interface capability, in the future.

### 3.1 Ingredient base

Colloid science and technology is broad based. Aligning this with an assessment of the ingredient base supporting these sectors means that a road map can only offer, in the main, general areas of potential activity. It is an area that has been extensively surveyed by a number of organisations and where possible IMPACT will seek to collaborate with these organisations.

In particular, a number of other Faraday Partnerships will have surveyed the ingredient base in areas specific to their market/technology sectors. Again IMPACT will aim to collaborate and pool the ‘information resource’ to produce a cohesive picture.

In each of the sections below, specific themes are described which have been distilled from feedback from company visits, consultation events and reviews of current capability. They have been written in a general sense rather than being tied to specific industrial sectors, but reflect the relevance and application of the theme to a number of industries.

#### **3.1.1 Easy/reliable ingredient substitution**

Crop-based renewable resource feedstocks: Crop-based renewable raw materials include oils from oilseed crops, starch from maize, tapioca and potatoes, sugar from sugar beet and cane, and cellulose from straw and wood. They are converted, via physical, chemical or biochemical processes, into chemical intermediates, such as polymers, lubricants, solvents and surfactants, for which, since around the 1940’s, petrochemical-based fossil fuels have traditionally been used as feedstock.

The US Department of Energy biorenewables road map suggests that by 2020, 10% of basic chemical building blocks will be from plant-derived renewables and this will rise to 50% by 2050. Current usage is <2% (2000). (ERRMA report ‘Current situation and future prospects of EU industry using renewable raw materials’).

The main drivers for renewables are preservation of fossil fuels, reduction in greenhouse gases and potential governmental green legislation. The overriding driver, in the absence of legislation, is undoubtedly cost.

The drive to exploit the use of crop-based renewable resources varies from continent to continent.

The drive to exploit the use of crop-based renewable resources varies from continent to continent. For example, in the USA 'the Clean Air Act' is predominant, while in France it is the use of set-aside agricultural land, and in Germany the 'Green Consumer Economy'.

As with current use of petrochemical-based feedstocks, the need for fuel will dominate (with gasoline production accounting for >90% naphtha being one example).

One main activity in this area is the development of biodiesel (methyl soyate). This has been actively investigated for over 10 years, and while this is set to continue, little impact is currently being made. It is worth reflecting that the life of oil has been significantly extended in the last few decades (oil was due to run out in the 1980's as seen in the 1950's) with better discovery and extraction methods. The latter has been significantly aided by colloid SET (cf. surfactants in tertiary oil recovery).

No doubt, even incremental improvement in surfactant-based recovery technology (let alone discovery of new fields) will affect the timing of replacements. Consequently, this is set to continue as an active research area for the foreseeable future.

The use of renewables will not be driven by formulation industries, but will adapt as they become available from bulk needs (particularly fuels). Cost of replacement will be the dominant factor given equivalent property performance. However, proposed EC legislation 'Sustainable use of chemicals'<sup>1</sup> may change this. Suggested deadlines are for substances exceeding a production volume of:

- 1,000 tonnes – at the latest by end of 2005
- 100 tonnes – at the latest by end of 2008
- 1 tonne – at the latest by end of 2012.

This may restrict the availability of a number of commonly used formulation ingredients as this legislation will make their production (registration) uneconomic so forcing recipe change.

Changing a raw material can have a profound effect on final product form unless the replacement is 'identical'. Different trace impurities or different levels of the same impurity will have unquantifiable effects. Continued underpinning research activity with trial alternative ingredients is a likely consequence.

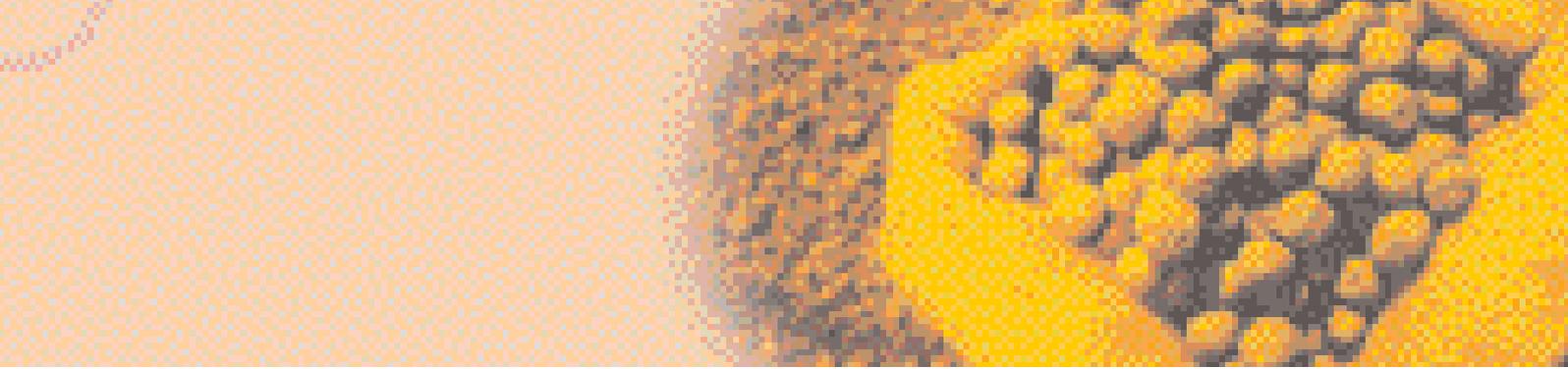
What is key in substituting renewables for petrochemical-based ingredients is that they offer alternate and/or improved properties, such as biodegradability, and/or new functionality. However, the effect of variable supply needs to be considered. Variations from the same source due to climate variations or different growing medium (cf. grapes to wine) need to be considered. Such variation might be overcome by fine-tuning of formulations based on a combination of rapid analysis and predictive modelling.

The ICI Company, National Starch, already markets biodegradable packaging based on starch from maize. As a result of the decision of the EC to harmonise its member countries' packaging regulations, Eco-Foam has been recently launched in Europe.

Renewable and hybrid replacement surfactants are in current use (for example, alkyl polyglucosides) which usually behave in an identical manner to more traditional alcohol ethoxylates, and can, in many instances, be used as a direct substitute offering a 'greener' product. Natural polar oils (for example, oleates, triglycerides) and perfume oils (for example, cineole, eugenol) are being increasingly used in combination with surfactants, replacing non-renewable mineral oils.

As noted above, prior to the petrochemical revolution in about 1940, ingredients in formulated products were dominated by renewables. An historical survey may help predict the future.

<sup>1</sup> <http://europa.eu.int/rapid/start/cgi/guesten.ksh> 'Commission sets out the path towards sustainable use of chemicals' Press release IP/01/201, 13/02/01.



### Life cycle analysis:

The concept of replacing petrochemical-based ingredients with renewables should not only consider the environmental benefit but the effective Life Cycle Analysis of environmental, economic and social factors. Modelling will certainly be influential in developing this concept further. Farming subsidies at present make renewables potentially competitive relative to petrochemical-based materials, but uncertainty in the policy of subsidies may be influential.

### Biological processes:

**Fermentation** – Use of fermentation technology will increase, but as with crop-based renewables, it is not likely to be driven by formulators' needs.

It is also likely that research in this area will be driven by higher added-value product applications.

Notable bioprocess developments include the Cargill Dow polylactic acid plant and the proposed (2004) DuPont 1,3-propandiol facility. Both processes use maize starch as feedstock.

Since the mid 1970's, Brazil has been using ethanol derived from sugar cane for automotive fuel. Approximately 13 billion litres is annually produced, which fuels around 3 million straight ethanol vehicles and 10 million 75% gasoline/25% ethanol vehicles.

Biopol (poly(3-hydroxybutyrate), produced by fermentation of the naturally occurring bacterium *Alcaligenes eutrophus*, was initially marketed by ICI with the expectation that it would become a multithousand tonne biodegradable plastics (packaging) business. This did not happen due to price and performance comparison with conventional materials such as polypropylene. The technology was sold to Monsanto and then on to Metabolix. It is likely that Biopol will find niche markets in, for example, speciality coatings and medical applications such as dissolving sutures.

### Organic to aqueous-based formulations:

This momentum to replace organic solvent based by aqueous based formulations, which was pioneered by the paints and coatings sector, is set to continue. Legislation and environmental pressures will force even small volume formulations to reduce the total amount of volatile organic component. Research into alternative hydrophilic compatible ingredients is an ongoing requirement.

**Enzyme Catalysis** – Wider use of enzyme catalysis in conventional petrochemical processes such as oxidation could have an impact on material supply, and much research is being conducted in this area.

### 3.1.2 Components' physical form

#### New crystal forms/polymorphs:

Polymorphism denotes the existence of more than one crystal structure of a substance. Different polymorphic structures of a material can, and do have, different physical, chemical, biological or pharmaceutical properties. While polymorphism has been recognized for 175 years, there has been little concentrated effort to study the fundamental phenomenon, its causes and its manifestations. Most of the research on polymorphism has been carried out in isolated centres on different theoretical and experimental aspects of the phenomenon. Key targets include:

- (a) developing capability for predicting the existence of particular crystal structures and their potential application from theoretical principles; and
- (b) providing (robust) routes for synthesis.

Polymorphism is an area in which Europe has more expertise than either Japan or North America.

#### Nanoparticles:

Nanoparticle technology is, without question, one of the 'hot' topics of research at present and for the foreseeable future. It has been described as the 'genetics of the material world', and the synthesis, characterization, optimization and processing of consistently sized particles will change the whole character of product performance in many industries.

“Nanoparticle technology...is described as the 'genetics of the material world.'”

IMPACT is at the forefront with the ACORN (A Collaboration On Research into Nanoparticles) Foresight LINK programme. Key requirements are not simply preparation of nanoparticles, but keeping them nano and scaling-up to commercial quantities. A possible alternative is their generation at point of use, so the nanoparticles are immediately incorporated into the final product like, for example, a polymer composite.

It is probable that new processes involving supercritical fluids, spinning disc technology and fine-tuned aerosol reactors, will need to be developed in parallel with product development to take advantage of these performance benefits.

New surfactants may be required to stabilise dispersions, and advances in analytical science to measure at the nano-scale will need to keep pace. Interestingly, nanoparticles are themselves being used as substitutes for surfactants in stabilising emulsions by providing a physical barrier. Advantages include no foaming and chemical stability.

Furthermore, nanoparticles are already being successfully used in consumer products such as sunscreens, and nanocomposite materials to replace metal air-intake covers or engine covers in automobiles (weight reduction and higher temperature performance). Drugs and agrochemical active agents, reduced to nanoscale level, show a dramatic increase in solubility and consequent improvement in ability to be absorbed.

Predictions in timescale for entry of new products based on nanoparticles in most cases are probably optimistic. However, the current high level of research activity worldwide should present a range of interesting options. Key application areas include speciality dyes for security (for example, fraud protection), drug delivery systems, fuel cell components, hydrogen storage devices and future quantum computing.

The USA and Japan are undoubtedly leading in this area, but Europe has a good position, and the UK is making a substantial contribution, although probably not funding at a sufficient level. IMPACT should continue to take a lead role in support of this area of technology.

A major potential problem is Health and Safety implications of nanoparticles. Clearly test protocols need to be developed. However, the power of the popular press to influence acceptance of this technology should not be underestimated (cf. GM foods).

### 3.1.3 Product robustness (storage, manufacture, performance)

Predictive tools:

Predictive modelling came through strongly during the strategic review exercise. Relevant questions included:

- What happens if an ingredient is changed?
- Can the interactions in a formulation be modelled to predict, for example, shelf-life stability, effects on final physical form (for example, rheology)?
- Can laboratory measurements, coupled with modelling, be used to predict final form manufactured product?

This is an area worthy of increased research activity.

There is good existing knowledge in the pharmaceutical, and the paint and coatings sectors, but this knowledge is not well established in other sectors. Awareness of what is possible needs to be highlighted. Increased computing speeds, combined with rapid experimental input to allow iterative development, will gradually provide increasingly robust models. Use of High Throughput Screening (HTS) in formulation development may be a route to rapid experimentation.

A variety of skills is needed to develop this area including modellers, physical scientists (synthetic/material/analytical) and engineers. Multidisciplinary programmes are an area where the UK is weak relative to many developed economies, particularly the US and Western Europe.

Replace all animal testing (cosmetics):

Work on cosmetics falls into two main areas:

- safety including fit for use, and allergic response; and
- efficacy including performance characteristics such as the effect on skin topography, formulation elasticity.

The UK prohibits testing cosmetic formulations or chemicals predominantly/exclusively used in cosmetics on animals. This restriction will soon be extended to apply across the EU.

However, other territories, notably Japan and the USA, still accept animal testing in order to substantiate safety for cosmetics to be launched on the market.

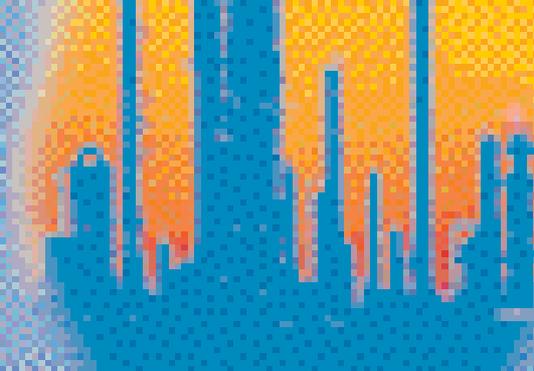
There are attempts to assess formulations based on knowledge of individual components. A potential problem here is the effect of 'combination toxicology'. Alternative tests to the use of live animals are being developed, for example, the response of skin from dead animals, the skin having specific property criteria such as age and elasticity, and using in vitro techniques such as cell cultures or skin reconstructs. Synthetic analogues of skin are also being pursued. Whole body modelling is a much longer term aim.

In summary, likely key areas of research activity to meet these identifiable needs are collated in Figure 3.



Figure 3: Summary of "Ingredient base" Research Themes

Perceived needs in Ingredient base	Short Term Delivery	Medium Term Delivery	Long Term Delivery
<b>Easy/reliable ingredient substitution</b> Crop-based renewable feedstocks:  Bioprocess:  Aqueous-based formulations:	Opportunistic use  Create intelligent database  Use of modelling capability developed for pharmaceutical sector	Legislation will accelerate introduction (1 tonne chemical production volume to be registered by 2012)  GM for enhanced specific ingredient yield becomes important  Use of modelling to predict effect of ingredient substitution increasingly powerful  Use of biocatalysis increases	Bio-diesel becomes viable
<b>Components physical form</b> New crystal forms/ polymorphs:  Nanoparticles:	Much experimental activity – new uses for "old" materials  Fraud protection Process routes explored	Predictive models  Drug delivery Fuel cells Scale-up becomes viable	Quantum computing
<b>Product robustness (storage, manufacture, performance)</b> Predictive tools:  Replace animal testing:	Use of artificial skin	Increasingly robust models developed as link HTS with faster computing  Continuously improving skin models	Whole body models
	Continuing drive to replace organic solvents by water		
	Safety protocols to be developed		



## 3.2 Product manufacture

In colloidal systems, there has always been a considerable effort expended in order to manage the manufacture of multiphase products to obtain a reproducible product. Any preparation of colloidal material also had the usual manufacturing requirements of a process with a minimum of steps, rapid, simple equipment, easy to use and clean, and robust in the sense of product specification. To this end the requirements in future manufacturing processes are unlikely to change, except that the degree of product complexity will add to the manufacturing burden.

In this section, the changes in materials and their functional form are addressed with respect to the method in which they are put together as a manufactured product. A greater emphasis on nanotechnology in the future, and therefore a more complex but specific arrangement of components in the different phases, clever manufacturing methods and techniques are required. Whilst this may be self-evident, it is also of great importance for future manufacturing processes that the progress of the product within the process is monitored. With this in mind, it is necessary to develop suitable measurement techniques to fit with the production methods.

### 3.2.1 *Process robustness and flexibility*

Manufacturing robustness and flexibility is a generic problem across all industry sectors and technologies. The route to a more robust manufacturing process is through greater understanding of the events taking place within the process by monitoring and predicting behaviour.

“Manufacturing robustness and flexibility is a generic problem across all industry sectors and technologies.”

One major task within this remit of producing sensors is the sensitivity to the very large range of sizes involved. Consideration of a nucleation and growth process will highlight this problem. The start is a collection of molecules and the finish is perhaps a 2 micron particle. A 1 Angstrom molecule, nucleating at 2 nm diameter, and growing to a 2 micron diameter particle represents a  $10^4$  increase in surface area, a  $10^6$  increase in volume and a collection of  $22 \times 10^9$  molecules. Sensitivity over this range is required for full control.

#### Monitoring in processing:

Any given material as it is prepared needs to be monitored through the process. Sensors and detectors need to be developed which are able to monitor various attributes of the material in “real time” and which can be applied “on line” or within the process. Additionally, because of the need to be efficient in manufacture, it is highly likely that any material will be produced in concentrated form bringing additional challenges, such as optical density and high viscosity, which limit some of the current methods of analysis.

Furthermore, the attributes that may be required may not simply be particle size but also particle shape and particle or droplet anisotropy. Particles may not simply be homogeneous or spherically symmetric, as core/shell particles are, but could be elongated with a different constituent along the length of the particle. For the process sensors to be truly effective, it is anticipated that they would provide information so that corrective remedial action could be taken in real time during the process. This would be the highest level of detection and output. It is also envisaged that at a lower level, a measurement-only system would provide useful information but would be a stage en route to a higher level system.

### Predictive behaviour:

One major problem of manufacturing colloids, particularly emulsions, is having the ability to predict the behaviour of the materials in the process which links in strongly with product design for performance. Having predictive modelling capabilities will not only give a powerful aid in scale-up of processes, but also in the original design and development of the process to produce a particular material.

A reasonable starting point for this type of activity is to produce a set of predictive steps that could be envisaged as a modular process. Although at present, there is a tremendous amount of information available to use as a base data set, there is equally a very large number of different process variables applied to a large number of processes. Attempts at deconvoluting this set of information may prove fruitless.

As a simple example, the emulsification process using only one stabiliser can be considered. The shear regimes involved vary considerably and change throughout the process as emulsification proceeds. The rates of transfer to and from the liquid/liquid interface are of paramount importance, and are to an extent the result of the local flow regimes, whether turbulent or laminar.

This argument suggests that a different starting point is adopted to understand, and consequently model, the behaviour of materials in the manufacturing stage. Naturally, this type of predictive modelling is also necessary when designing the ingredient base, as identified within the section on predictive tools.

### Modular units:

Modular units as suggested above may be a method of producing an overall understanding of behaviour in a manufacturing process. They do however have a greater utility. The use of modular units gives greater flexibility to a manufacturing unit. Each module would be well understood since it is linked in with a predictive modelling package. Here again sensors and detectors would be a key part of the technology.

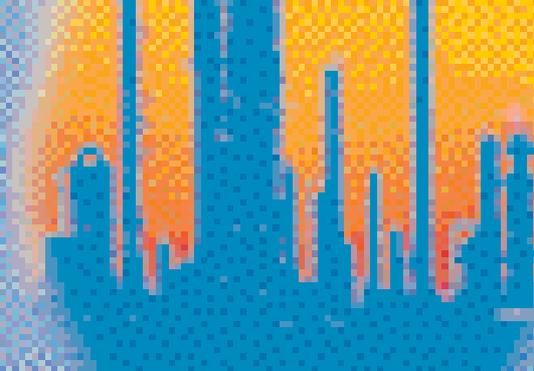
### Continuous process:

Many processes are "one pot" preparations which would be a 'holy grail' for any process, but it is not unreasonable to imagine a continuous process where one module (from above) feeds directly into another module, the second stage of a process, and so on. As with emulsion polymerisations now, a semi-continuous process can be seen as the second stage to one pot production. This has value in maintaining a flexible manufacturing capability, whilst adopting the (semi-)continuous process.

### Small scale:

It is noted that for some niche markets that require high added-value materials, there is no requirement for large quantity manufacture. In this respect, the idea of having an understanding of both batch and semi-continuous processes is still of high value. A flexible approach to small scale manufacture is facilitated by use of modular equipment. The links to gaining understanding of small batches to develop larger scale processes to the assembly of multicomponent products and delivery on demand for distributed systems is clear.





### 3.2.2 *Smart assembly of multicomponent products*

This capability is a direct approach to the manufacturing challenge for producing process engineering with well developed and understood scale-up rules. Smart materials constructed from colloidal or nano particulates have their added value in the arrangement, or organisation, of the particles as a 3D assembly. There are two fundamental approaches – top-down and bottom-up. Top-down is a method of moulding or reducing bulk materials by, for example, lithography or milling. Bottom-up is a chemical method to build clusters, particles and structures.

Within the area of controlled chemical approaches is the use of assembled templates to control the architecture at the nanometre scale. Examples of structures may range from simple spherical particles of a given property arranged into an average nearest neighbour position and held in a gel, to much more complex systems. Lyotropic phases can be used to template metals, alloys and metal oxides.

Alternatively, monodispersed spherical particles can be assembled into arrays which can be deposited onto electrode surfaces from which it is possible to template electrochemically deposited metals, alloys, metal oxides, semiconductors and polymers. Removal of the template spheres produces inverse structures. These all have properties that depend on the sphere void size and film thickness, which in turn controls the optical, electrical and magnetic properties of the material.

“ Smart materials constructed from colloidal or nano particulates have their added value in the arrangement, or organisation, of the particles as a 3D assembly.”

The materials constructed in either of these two ways will find use in electrocatalysis, sensors, energy conversion and storage, separation and electroanalysis.

The question of scale is one that is now difficult to define for materials in their construction. At the molecular level we are predominantly involved with product design to create larger 3D structures from assemblies of molecules into, for example, nanostructures and nanoparticles. It is not inconceivable that a continuous process from molecules to fabricated engineering materials could be carried out in a single process or as a connected set of processes. For instance, self-assembly at the molecular level can be manipulated to form self-assembly at the nanoscale and so on. This strongly links with the controlled 3D architecture in product design so the distinct and separate manufacturing process, that we might have classically called the fabrication stage, is now inextricably linked with construction of the nano- and micro-components themselves. In developing the themes within this section, this increase in scale has been considered.

#### Direct control of the assembly of components into 3D structures:

The construction of a material at the small scale offers new opportunity for effects. The first level of this effect is the nano- or micro-component. This theme is dealt with in a parallel section in Product Design – controlled 3D architecture. However, in order to develop the route to manufacture it is also necessary to consider it in this section.

One example of this type of approach is the specific placement of components in core-shell structures. This is not new to the emulsion polymer field where many core-shell particles have been produced. Moreover, there have been products designed and produced during the past two decades which have reproducible particle structures, and which are multicomponent, but yet are not homogeneous or radially engineered (core-shell).



An example is emulsion polymerised multilobed polymer composites that impart unique film-forming properties or rheology control. Within the materials, each lobe was constructed from a different polymer material. It can be envisaged that this built-in inhomogeneity could find use when aligning a particle in an applied field such as electric, magnetic or gravitational for instance. Of course, it is entirely conceivable that the field effects themselves can be used as a route to the manufacturing technique.

As a part of this technology, the alignment of high aspect ratio components in composite materials and structural materials could be considered. It is tempting to suggest that the imposed field in this case would be a flow field, shear or extension. Work in this area to date has had limited success.

Similarly, there are currently many attempts to encapsulate materials and these include inorganic materials as well as polymer-based products. Although these materials can be products in their own right they can also be considered as a precursor for a truly 3D arrangement of individual particles for the actual required material.

#### New ways for continuous processing:

In attempting to take a view of new methods for producing continuous processing in order to make materials, there are clear generic changes that can be adopted on existing processing techniques before more imaginative or speculative methods need be developed.

The major reasons for adopting a new process are if either a particular material cannot be manufactured with current technology, or if there are considerable benefits from changing the process. Given the current and perceived continued future drive towards nanotechnology, the former would appear to be the more likely given that manipulation of nanocomponents into large 3D structures will require methods and techniques which are not currently available. Whilst not attempting to be prescriptive in the way in which this can be progressed, there are some approaches that may readily lend themselves for adoption.

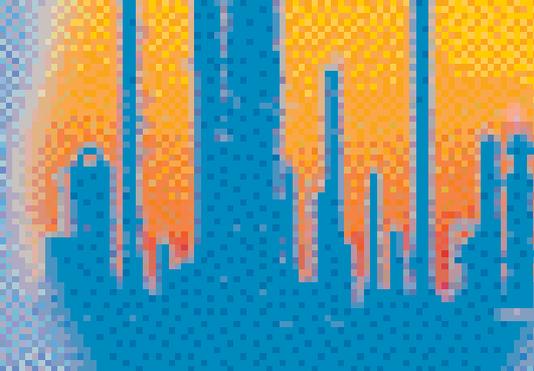
The use of film technology, where transfer from reel-to-reel in building complex 3D structures, has potential. The method could be readily adapted for putting components together in a sandwich form, for example, as a route to building complex circuitry. In addition, with appropriate control and process monitoring, use for building nano-structures can also be envisaged. This would lead to 3D materials having manufacturing capability with control at the molecular level, for example, for cost-effective manufacture of smart materials.

#### High quality specification:

In the design of a product, attention to the specification of the components, that is, the raw materials, and their variability, is critical. This is also true of the manufacturing process, and the effect of the raw material variability in the process, and thus on the final product.

“In the design of a product, attention to the specification of the components, that is, the raw materials, and their variability, is critical.”

There are two routes to effectively handle this problem. The first is to ensure that raw materials are supplied to exacting standards and the manufacturing process as a result need not be responsive to variations. The second approach would be to develop flexible process plants with rapid process control to respond to variations in raw material quality. This is described earlier in this section. The latter approach would further lend itself to a switchable process which could also be used for flexibility of manufacturing. In this way, there is a design link from colloidal materials to product application process.



Again the route to being able to cope with the constraints on manufacturing as described above will rely upon having adequate monitoring capabilities. Sensor technology will therefore be an implicit component of developments in manufacturing technology. Detection of a material specification parameter may also include a sensor technology different to a probe for a physical property, but which could also be a chemical or even biological property.

### **3.2.3 Distributed facilities**

“Distributed facilities” means the ability for a process to be either portable in the sense that it can be delivered to sites remote from a centralised organisation, or easily and cost-effectively available at point-of-use. In the sections above, ideas for technology development have been described. Some of these ideas can be incorporated into approaches for distributed manufacturing methods. A brief summary of a set of approaches appears below.

#### **Portable manufacturing to access globally diverse markets:**

The concept is to facilitate a manufacturing capability that allows identical units to be placed globally in order to allow local production quality that is predictable, cost-effective, reduces distribution costs and allows production on demand. There are naturally strong links into modular units and linked modules for flexibility described above, and strong links into the need for robustness and flexibility in process engineering.

#### **Flexibility of plant design:**

If a truly predictive model of manufacturing plant is available, the design of a one-pot process should give the required product properties. Alternatively, flexibility of processing may be better served by a modular approach, but the design still requires a predictive model for a successful manufacturing process.

#### **Delivery on demand:**

Development of systems capable of delivering complex colloidal formulations at the point of application now becomes more than simply a flexible, portable global manufacturing capability. This embodies the concept that material can be produced on demand at the point of application.

Consider for instance the drop-on-demand process used in ink jet printing. If the process used only the raw material ingredients input into the equipment, and a drop with the correct printing properties (electrical conductivity), colour (pigment type), intensity (concentration and particle size), polymer film former (curing properties, abrasion resistance and mechanical integrity), viscosity (rheology defined by the polymer and particle concentrations) and drying properties (solvent type, maybe water based) could be produced, this would give maximum flexibility to the process and be available at the point of application in a variety of forms. To an extent, this idea is currently being used in the paint industry in the point-of-sale colour matching devices. However, these devices are not vastly flexible, nor sophisticated, but they do exemplify the type of system which could be developed.

Other examples of the utility of this flexibility exist, and a good example is that of the application of agrochemicals. There is a clear need to apply specific formulations to only those plants that require it and in the correct dose. By having a number of different treatments available at the point of delivery, a smart system would be able to select the correct herbicide or pesticide for the job, as well as the correct dose, and apply to only the identified area.

Since in agrochemical application it is highly likely that several active ingredients would need to be applied simultaneously, the smart system would also recognise those active ingredients to be included into the complex formulation that would be generated at the point of application. It is easy to imagine that this same capability could in principle be applied to many applications including pharmaceuticals for ‘formulating’ at the point of administering.

In developing this type of technology capability, it is clear from previous discussion that it is imperative that the materials are monitored during the process. The need for point of use diagnostic sensors and detector devices is a clear requirement, in line with the same requirement for personalised products, as identified in “Customer expectation” research themes (section 3.5.4).

### **3.2.4. Process efficiencies**

It would normally be assumed that any manufacturing process would be designed with efficiency in mind. There are of course many different ways in which the process efficiency needs to be considered, but it is not the remit of this text to consider these. These would be expected to be a part of any work conducted under the principle of designing a robust and flexible process.

However, there are some features that are worthy of consideration, and these rely on the idea of having the ability to monitor and be reactive in the process. It is also worth noting that, as with high quality specification above, reactive processing may not be adequate, and proactive processing relying on pre-process sensing may be required. Evaluation of this principle as a viable option would be useful.

#### **Remote sensing:**

Remote sensing, that is, the device is remote from the operator or is in an inaccessible zone of the process, is already widely available for properties such as temperature and pressure, but much less advanced for measurement of colloidal properties. In-line, robust, non-perturbing sensors are likely to require creation of microstructures often based on nanostructure components. Processing “submarine” detectors held within a reactor could make the same type of colloid property measurements. The submarine idea has a current large scale analogue, that is, the use of down-hole sensors in the oil drilling industry.

To consider this analogue more closely, it would be of enormous value were these remote sensors capable of making rheological measurement which could be used to determine colloidal microstructural information and relaying this information rapidly for corrective process treatment. There is a clear need to develop new sensors and understand the correlations between rheology and microstructure.

In summary, likely key areas of research activity to meet these identifiable needs are collated in Figure 4.



Figure 4: Summary of “Product Manufacture” Research Themes

Perceived needs in Product Manufacturing	Short Term Delivery	Medium Term Delivery	Long Term Delivery
<b>Process robustness and flexibility</b>	<p>Sensors and detectors for characterisation in-line or batch</p> <p>Modular processing</p>	<p>Process modelling for prediction</p> <p>Continuous processing, one pot</p> <p>Small scale</p>	
<b>Smart assembly of multi-component products</b>		<p>Direct control of the assembly of components into 3D structure</p> <p>Method development for bottom-up and top-down nano- and micro-properties to be scaled up</p> <p>New ways for continuous processing</p> <p>High quality specification</p> <p>Sensors and detectors</p>	
<b>Distributed facilities</b>	<p>Portable manufacturing</p> <p>Flexible plant design</p>	<p>Delivery on demand</p> <p>Process modelling for prediction</p>	
<b>Process efficiencies</b>	<p>Remote sensing</p> <p>Pro-active process control</p>	<p>Process modelling</p>	

## 3.3 Product design

This section covers the need for, and the ability to, manipulate product form to deliver product performance. This is a vital requirement in a wide range of industries. In the pharmaceutical industry, for example, the form in which a drug is delivered to the patient will determine where and at what rate it is released in the body. In the detergents industry, the release profiles in the wash of the components of a fabric washing powder are controlled by manipulation of product form.

Key elements of product design are the ability to produce specifically designed structures, the ability to control shelf-life and the ability to control the delivery of the key benefit at the point of use.

For all of these applications, there needs to be clear and controlled correlations between bulk property and microstructure. Key elements of product design are the ability to produce specifically designed structures, the ability to control shelf-life and the ability to control the delivery of the key benefit at the point of use.

### 3.3.1 Predictable product stability

The overall goal is intrinsic stabilisation and design of the product from the outset. Specific elements of this are explained as follows.

#### Improved modelling techniques:

There is a need for models of the ageing process to enable product stability to be predicted as a function of, for example, formulation components, and time and conditions of storage. In the short term, any such models are likely to be formulation specific, for example, to predict stability of a paint or a household cleaning formulation. A longer term goal would be to make the models more generic.

In many industries, products are required to have shelf lives of around two years. Intrinsic to developing models of long term stability is the ability to measure small short term perturbations to the product properties, and to be able to extrapolate these to longer storage times. This may in turn require development of improved measurement techniques.

A longer term goal therefore would be a new detection system to monitor stability that works for all products rather than being specific. Developments in ultrasound scanning and interpretation of multiple scattering are promising, but not yet at a stage for wide scale usage.

#### Improved processing techniques:

In addition to choice of formulation components, the choice of processing route has a major influence on product stability. There are many examples of cases in which the best formulation possible is not stable unless it is processed in the optimum manner, so the formulator must work closely with the process engineer to optimise process route and conditions. See below “Link to manufacture process and product performance” (section 3.3.2).

As an extension of this approach, an elegant solution to product instability is to make the final product at the point of use so as to avoid any issues of instability. This technique is already applied in many industrial applications, for example two-pack polymer systems.

#### Generic solutions:

The target here would be generic solutions to stabilisation problems rather than the specific solutions discussed above. A ‘holy grail’ would be a universal stabilising solution able to address all dispersion problems. By definition, development of such technology must be seen as long term.

### 3.3.2 *Link to manufacturing process and product performance*

In many cases product design is limited and restricted by constraints imposed by the manufacturing process, whether this is because of limitations of existing process technology or limitations of existing plant capability. Research into the following areas would be beneficial in reducing the dependency of design on processing:

- Improved modelling of manufacturing processes enabling identification of the key process drivers of product design, and then defining predictive models to allow optimisation of both design and process. Initially progress is likely to lead to models of specific product types but more generic modelling would be a valuable longer term target. It is likely that improved sensors, and other measurement techniques, will be required to allow accurate in situ monitoring of process variables in real time.
- Development of more flexible and modular process plants – this is discussed in more detail in the section on ‘Manufacturing’.

### 3.3.3 *More efficient products*

There are many constraints being imposed on existing products by the developing/emerging external drivers such as need for a cleaner environment, need for safer products and need for lower costs. Changing consumer lifestyles and demographics are also demanding more efficient products. There are also many emerging new technologies (especially in the biosciences area) that are already providing, and will in future provide even greater, opportunities to develop and deliver more efficient products.

#### Low environmental impact:

This issue is discussed in more detail in the sections on ‘Consumer expectation’ and ‘Product performance’. Some specific examples of where this impinges directly on product design are:

- Finding a way of achieving the desired end effect with less ingredients/components by a more rigorous understanding of the basic formulation and their interactions. This in turn will require robust and flexible modelling of formulation physical chemistry, product delivery and the chemistry of the interactions between the individual formulation components
- Components having multifunctionality that are tuneable to the desired performance. This builds on the item above in that it should facilitate a reduction in formulation complexity. Multifunctional components would be a first step, for example a surfactant able to deliver cleaning, water softening and fabric care. However, much more valuable would be a facility to tune the function of the formulation component to suit the desired application process or end benefit required. Another option would be to design enzymes with multifunctional sites on one molecule.
- Novel systems that allow the avoidance of non water-based solvents. This is becoming vital for very many industries as the pressure grows to reduce volatile organic carbons (VOCs) such as solvents and delivery devices.

#### Smart effects:

There would be huge advantages in being able to design systems that could interact with their environment.

Examples of goals would be:

- The ability to be able to reduce chemical load by ensuring a targeted delivery of ingredients in a given application.
- In situ generation of transient ingredients to improve efficiency at reduced loading. This would be of immense interest in many fields including medical, agriculture, domestic and industrial cleaning.
- Systems which degrade to harmless effluent once the benefit had been delivered.

The section on product performance discusses smart effects in more detail.

### Controlled release:

There are very many applications in a wide range of industries where the ability to control the delivery of key ingredients is a vital part of product delivery. Examples include the segregation of incompatible ingredients up to the point of delivery, and their release at exactly the right time and/or place for the given application. The essentials are delivery of the right product at the right time and place at the correct concentration. Improvements over current technology will come from development of techniques to build controlled molecular architectures – this is discussed below.

#### **3.3.4 Microparticle design**

The requirement here is to be able to design and make nanoparticles with specific and controlled properties. The ability to be able to reproducibly control the size and shape of nanoparticles, and to produce very narrow particle size distributions will lead to greater control over performance and stability. This control will be even greater if we can achieve the ability to prescribe the surface properties, chemical properties, surface roughness, porosity and permeability of the individual particles. Surface modifications of the nanoparticles will allow control of functionality. Design at this nanolevel will require the ability to manipulate materials at the atomic level – this is a new technology that could lead to new science.

#### **3.3.5 Controlled 3D architecture**

The requirement here is to be able to design and deliver specific product architecture. This could be as assemblies of nanoparticles in both solid and liquid formats, for example as thickened gels, films or more complex 3D constructions. Potential applications of controlled 3D assemblies are numerous and varied, for example:

- Control the porosity and surface chemistry of particles at the nanoscale to optimise catalysis performance.
- Controlled catalyst morphology – 100% efficient use of active sites.

- Manufacture of synthetic enzymes as miniature production plants without the issues of hygiene.
- Intelligent release of antimicrobials from surfaces.
- Means of controlling different morphologies of materials.

### Imaging of 3D assemblies:

To be able to properly construct 3D assemblies, it is necessary to develop improved methods of imaging. It is currently difficult to image nanomaterials, especially in vivo. One potential opportunity would be to develop X-ray lithography. Wider research on nanoscale imaging techniques should be supported.

### Manufacture of 3D assemblies:

There is currently little industrially-applied expertise in the ability to build controlled and reproducible assemblies of colloidal domain systems. Of particular importance is the assembly of nanoparticles into 3D arrays to deliver defined macroscopic structures with highly tuned properties. Potential routes requiring research to identify and develop their potential are:

Bio-routes – Nature builds extremely complex architectures – we need to be able learn from and mimic this. There should be enormous opportunities from a combination of biosciences and colloid science expertise and techniques.

For example:

- Using enzymes as production plants
- Self-assembly using immunological knowledge
- Bioorganisms as building blocks for materials
- Role of colloids in cell recognition
- Polymer-based gene delivery systems
- Surface chemistry-protein conformation-cell responses
- Novel antimicrobials

Nature builds extremely complex architectures – we need to be able learn from and mimic this.”



Molecular templating – The requirement here is for structural assemblies that can act as templates for the controlled building of colloidal structures. There is a clear science gap in the understanding of molecular templating/assembly processes. Potential routes to such templating could include thin film and optical templating (so-called optical tweezers), electrophoretic or optical field as frameworking devices, nanoscale, macroscale, thin film or print on textiles, crystal growth modification, development of new surfactants for colloid formation, and the uses of polymers and foam structures as templates.

For all of these, studying the disassembly could provide information on the assembly.

Self-assembled systems – This builds on the concept of molecular templating but is more elegant because the controlled architecture would self-assemble. This is conceptually similar to the way in which a crystal first nucleates then grows in a tightly defined structure. Many biological systems could be said to self-build and it is here that research could lead to promising routes.

Improved measurement techniques – Controlled assembly of colloidal domains will, of necessity, require processes for measurement and feedback on a nanoscale. This in turn will require improved techniques for the visualisation of the assemblies, and for sensors and measurement devices to monitor the assembly process. Modelling of the assembly process is also likely to pay huge dividends.

Process engineering – Design of controlled assembly and production, even at the scale of “test tube” quantities, will be a major challenge. Beyond this, scale up to an engineering process will be a huge challenge – this is discussed elsewhere in this document.

### **3.3.6 Design link to product application process**

Another key input to product design is the limitation often imposed by the product format. For example, a product that might be relatively easy to design in the format of an aqueous solution, but may be very difficult to produce as an aerosol or as a powder. In many cases, accurate specification and control of product rheology is required to optimise product delivery in the format needed by the end user. Research goals to facilitate such design are:

- Improved understanding and modelling of the effects on the core formulation components of the additional materials required to deliver that formulation in the desired format.
- Improved understanding and modelling of the effects on the core formulation components of the manufacturing processes required to fabricate the desired format.
- Definition of routes to more robust formulations better able to cope with additional constraints of form at delivery.
- Improved methods of controlling the delivery of the core formulation in a range of formats.

In summary, likely key areas of research activity to meet these identifiable needs are collated in Figure 5.



Figure 5: Summary of “Product Design” Research Themes

Perceived needs in Product Design	Short Term Delivery	Medium Term Delivery	Long Term Delivery
<b>Predictable product stability</b>	Predictive modelling of formulations and processing		Modelling at molecular scale Generic formulation technology
		Measurement and sensor development	
<b>Link to manufacture process and product performance</b>	Improved modelling of manufacturing process Flexible plant		Generic models
<b>More efficient products</b>	Multifunctional ingredients Improved modelling and measurement techniques VOC-free water-based solvents Target delivery Delivery via transient species Controlled and triggered release		Tunable functionality
<b>Microparticle design</b>	Molecular design of nanoparticles		
<b>Controlled 3D architecture</b>	Nanoscale imaging techniques Bio-routes to 3D assemblies Molecular templating Process scale-up for 3D assemblies		Self-assembled systems
<b>Design link to product application process</b>	Modelling formulation – format links Controlled delivery versus format		

## 3.4 Product performance

This section is to define targets for research that will provide knowledge about the key factors determining product performance. Since this knowledge will determine the product design, there is likely to be significant overlap between these sections. In general terms, performance research will give us information on what is needed to build a product, and product design research will provide information on how to build the products.

### 3.4.1 Predictable performance criteria

At first sight this looks to be difficult to generalise, as the range of products across different industrial sectors suggest a plethora of diverse parameters relating to the product performance. However, it is possible to identify a range of properties that underpin performance which are common across a whole variety of products.

Other examples of generic questions underpinning performance of a range of product types include:

- a) wetting, coating or surface film formation: what processes govern: coherent film generation; development of structured, multilayer or phase separated domain thin films; controlled 2D assembly from colloidal domain structures or self-assembly of complex films
- b) emulsification or solubilisation efficiency: what are the key parameters to build into products to optimise, for

For example, the factors determining aerosol generation, and subsequent droplet impaction and wetting onto a target surface is important for a variety of very diverse products in a range of different industrial sectors. These include ink jet ink and paper coatings, application efficiency of agrochemical sprays onto crops, inhalation efficiency for either drug delivery efficiency or minimising product toxicology, and aerosol application for household cleaning products

In all of these cases, knowledge of the effects of formulation components on droplet break-up, surface impaction and wetting, and subsequent drying are key to optimising product performance. While much is known about some elements of these processes, there are some major gaps in the science knowledge base, for example, the nature of the surface being wetted or the phase structures created on drying. These need to be researched in order to be able to make robust predictions of the effect of composition on performance.

example, cleaning of skin, fibres, textiles, surfaces, porous materials; creation of stable emulsions or dispersions after point-of-use application

- c) efficiency of delivery to target: what factors in the post-application fate of effect chemicals, for example drugs, agrochemicals or biocides, can be optimised via the formulation vehicle, and what determines the effect of composition on active ingredient uptake, bio-availability or mass transport.

In most of these areas, the product performance is balanced against other design criteria, for example cost, manufacturability, safety, customer practice or convenience, and the real benefit would lie in the ability to measure key performance parameters in conditions close to real-world practice, or to be able to simulate or predict the sensitivity of these parameters to product composition and form.

The real benefit would lie in the ability to measure key performance parameters in conditions close to real-world practice. ”

### Mechanistic research:

In each of the examples above there are some clearly identifiable questions into the mechanisms underpinning certain aspects of product behaviour. Some of these are already understood, and the challenge is to relate the behaviour to product composition.

However, there are others, for example, dynamic behaviour of surfactants at interfaces which are not fully understood, partly because of limitations in techniques to measure dynamic surface tension at short timescales.

Similarly, understanding mechanisms of complex film generation is critically dependent on improving the current capability to monitor a variety of film formation processes, in real time, under ambient conditions with sub-micron length scale resolution. Proximal probe microscopy and developments in surface spectroscopy are likely to be important new tools in this area.

### Multifactorial statistical research approaches:

In many instances, the product performance is a very complex behaviour that is not readily amenable to traditional mechanism-based investigation. In these cases, there is very real value in the development of statistical experimental design and multifactorial analysis methodologies to identify the most important aspects of product composition underpinning the product performance. While these studies typically do not easily lend themselves to explaining the dependencies, they are nonetheless valuable in identifying and quantifying guidelines for product design.

### High throughput experimentation:

The use of multifactorial analysis to determine key dependencies can be greatly enhanced by an increased availability or high throughput experimentation. In addition, the ability to run a much higher number of experiments cannot only enhance the robustness of the statistical experimental design; it can also allow multifactorial experimentation to be used to investigate mechanistic aspects of a complex cause-effect relationship, where several mechanisms are operating on the system in an interdependent fashion.

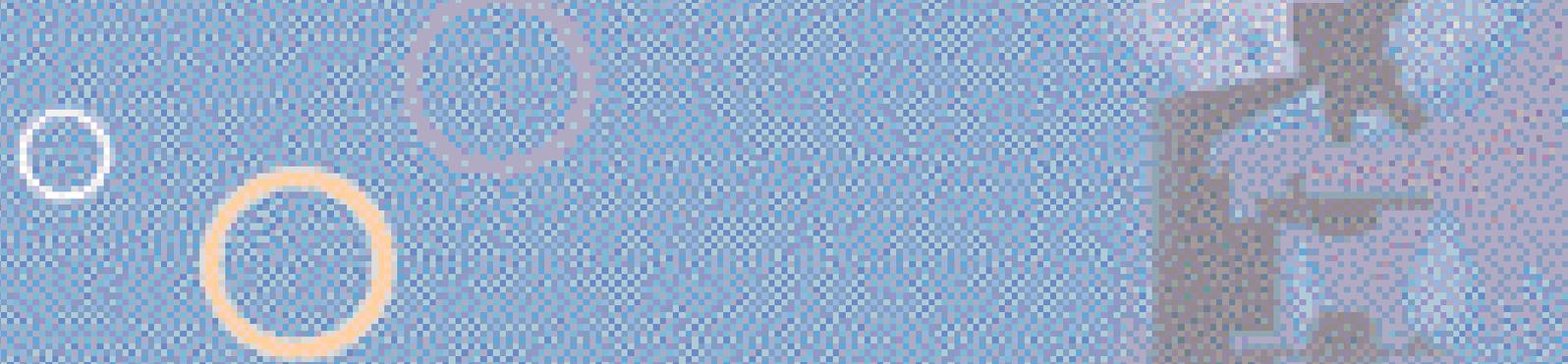
Application of high throughput technologies in this field will require significant development in both the "make" capabilities of currently available automation systems, particularly in dispensing solids and non-Newtonian liquids. It will also require a number of new developments in the "measure" capability to be able to monitor a wide variety of "material" properties. This required two key developments – the automation/robotisation of the processes, and miniaturisation of samples used for the process. The former is perhaps more readily achievable with incremental improvements in current technology, but the latter throws up significant challenges, for example, in obtaining "representative" samples/behaviour of multicomponent systems in smaller sample sizes.

A number of these issues are being addressed via the current EPSRC funding programme on high throughput technologies. It will be useful to ensure close dialog between colloid "user" communities and the research "provider" communities in this field, as there is enormous scope for research to develop new and enhanced capability.

### 3.4.2 Performance robustness

Research to deliver product performance robustness is about determining how to ensure the criteria for product performance can be met in the variety of real-world situations pertaining at the point of use of the product. The research outlined in the above section will be critical to delivering these targets, with the added caveat that the studies must also tell us which characteristics of the real-world applications are likely to be key in ensuring product performance is deliverable in a wide range of conditions.

In simple terms, this might be to ensure product stability (a topic comprehensively covered in the "Product design" section above) in a suitably wide range of climatic conditions to encompass global market and varied warehouse sophistication.



However, it is also likely to require performance operating over a range of other parameters critical to key aspects of the product performance as described above.

#### Quantitative prediction and modelling:

If there is good mechanistic understanding of a process determining product performance, for example as in film formation, this should allow generation of quantitative prediction or simulations to be developed which can be used to determine boundary conditions for acceptable product performance. The key is that the understanding must be sufficient so that these are truly quantitative in order to define precise specifications for acceptable use of products.

In many examples of colloiddally-determined phenomena, analytical mathematical expressions can be derived which are sufficiently quantitative to meet this requirement. However, the current limitations of molecular simulations regarding relatively small molecular populations and pico-second timescales are concerns for the development of computer simulation methods with the same degree of quantitative rigour. Given the speed of development of computational power and improved semi-quantitative modelling paradigms, this is an area which should offer interesting developments in the near to medium term future.

#### High throughput experimentation:

The alternative approach to determining robustness is to directly measure the desired end-effect (or a sufficiently robust laboratory simulacrum) over a much wider range of experimental parameter space than is available in traditional methods. There is enormous scope for this to be achieved if the improved “make” and “measure” capabilities outlined above can be achieved.

#### Controlled and triggered release:

Many aspects of performance robustness lie in the ability to segregate potentially reactive components of multi-component systems and/or allow them to become molecularly available under the appropriate conditions, so

greater application of cost-effective colloidal-domain controlled and triggered release systems is likely to be of increasing importance in this field.

There are many examples, as the following list illustrates: Encapsulation can be used to:

- reduce chemical degradation e.g. oxidation, reduction or hydrolysis in storage;
- trigger release in response to a change in an environmental variable e.g. pressure, shear, temperature, pH, ionic strength, light, hydration or oxidation (see section below);
- stabilise products against physical instability e.g. solubilisation, coalescence or crystal growth;
- target availability to enhance efficiency or reduce toxicity.

### 3.4.3 *Smart effects (i.e. stimulus-responsive systems)*

There are many aspects of product performance that could be enormously improved by development of systems that interact with the environment around them. The result might include: more efficient use of chemicals; increased specificity, for example, enhanced drug efficacy with reduced side effects; tailored physical property to match change in conditions, for example, responsive surfaces providing active cleaning or reduced friction/drag in a variety of flow conditions; self assembly-disassembly systems allowing ease of application or improved product recovery and/or recycling.

In addition to determining the appropriate stimuli for controlled and triggered release systems, likely research topics to provide the understanding of how to develop products of this type include:

#### Paradigms from biosystems:

Biological systems are an obvious example of stimulus responsive systems, so what can be learned from them for application in this field?



At a molecular level, the biophysics of proteins, both functional, for example enzymes, and structural, for example actin, is a very well researched field, and the generation of synthetic analogues to these systems, or the use of biotechnology to engineer purpose built biomolecules or biopolymers, is an exciting developing arena.

At a molecular assembly level, biomembrane structures are an example of self-assembled surface active systems which provide routes to exquisitely tailored interactive systems. At an informatics level, the rapid growth of genomic, proteomic and metabolomics is providing potential to translate molecular “information handling” physics into synthetic analogues.

Whole cell, whole organ or multicellular organisms are clearly the most sophisticated “smart” systems available as subjects of study to provide analogues for synthetic systems utilising colloidal scale physics to develop new approaches to novel products. It is recognised there could be great value in catalysing generation of cross-disciplinary think tanks in certain areas of smart system development.

#### Controlled assembly-disassembly:

There is an enormous depth of knowledge on the routes to generate, tailor and characterise colloidal domain systems. There is a deep and well established knowledge on the interaction of colloidal domain particles (gas/liquid/solid). However, there is relatively little sophisticated knowledge or application of knowledge to the self assembly-disassembly potential of colloidal domain systems with, perhaps, the exception of film formation processes. Even in the latter well-researched area, there are challenges to extend the knowledge and control available with micron particles to composites made from sub-micron particles.

As the nanotechnology revolution starts to generate functional entities with sub-micron scales, the ability to assemble these structures into ordered arrays or complex geometries, to deliver macroscopic devices or functional materials has enormous potential, and presents important research targets for the colloid community.

#### Smart surfaces:

These have been covered to some extent above, but there is a strong demand from a number of industry sectors to have a better understanding of the way in which surface morphology can be created and designed to change in response to conditions to enhance surface properties. Examples include: triggered changes in physical nature of surface such as switch from hydrophobic to hydrophilic, attractive-repulsive, controllable abrasivity/drag or chemically responsive nature such as self-cleaning, biocidal surfaces for household/industrial use, and textiles.

#### Polymer or composite electronics/photonics:

This is perhaps a more important topic in the design of products, but there are questions on the fundamental nature of composite materials that govern their electronic behaviour which require further fundamental research, particularly in being able to characterise, understand and then predict the importance of domain sizes and structures on the 1-100 nanometre length scale.

### **3.4.4 Low environmental impact**

This issue is dealt with more fully in the section on “Customer expectation” (section 3.5.2), but there are two aspects of understanding product performance in this respect which have been raised as being of strategic longer term importance.

#### Durability versus disposability:

It is felt that for many formulated materials, in product form or post-application form, there is value in determining the effects that contribute towards the balance between products that are sufficiently durable to fulfil their function, and sufficiently susceptible to environmental effects to be disposable and/or biodegradable in an environmentally acceptable form. There may well be value in having a greater understanding of the factors which impact on the “grave” end of the product “cradle-to-grave” analysis.

### Triggered degradability:

The increasing responsibility being levied against the manufacturer to ensure recyclability of products is felt very heavily in producers of multicomponent products, which includes, by default, all formulated products. The way in which triggered disassembly could be built into products is touched on as a target in the product design section of this report. However, it is also worth mentioning in this section the need to have a greater understanding how the real world conditions and variability of any disassembly process impacts on product performance and recyclability.

### 3.4.5 *Biocompatibility or bioavailability*

This covers two aspects of how effect chemicals interact with bioorganisms:

- a) optimising delivery of chemical to a biological target, for example, drug to enzyme or tumour, agrochemical to pest species or biocide to microorganism
- b) minimising non-target uptake, for example, reduced toxicology or user hazard.

The current level of understanding with regard to how chemicals interact with a whole range of organisms is an immense and complex task that is outside the remit of IMPACT research activity.

There are however some key areas where the formulation vehicle used to deliver a product, whether or not it is targeted at an organism, will be a key determinant of the bioavailability. Similarly, many of the materials developed to specifically interact with bioorganisms have to be designed to cope with interactions with tissues or whole organisms, for example, bioimplants, drug delivery devices, biosensors. In these areas, there are four key topics that have been raised as important research targets which do fall within the IMPACT remit.

#### Interfacial material properties determining interaction with biological tissue:

Cellular responses to implanted material, for example sutures, stents, prosthetic devices, biosensors, are critically

dependent on the chemical and physical nature of the implant surface. There is already a good body of knowledge on many key aspects of this interaction at a general level, but there is clear scope to understand these effects at a much more predictive level in order to manipulate the implant surfaces to control the interaction. Examples of this include, altering the chemistry of the surface and also the morphology, in cases where it is known that surface patterning plays a significant role in mediating cellular response.

#### Biocomposite or “bionic” products:

In addition, there is clear evidence that biocomposite materials incorporating complex functional biomolecules, cells or cellular assemblies are being developed as new product concepts. The ability to design, manufacture and stabilise such products will place increasing demands for greater predictive scientific knowledge on biomaterial-synthetic material interactions.

#### Formulation effects on bioavailability:

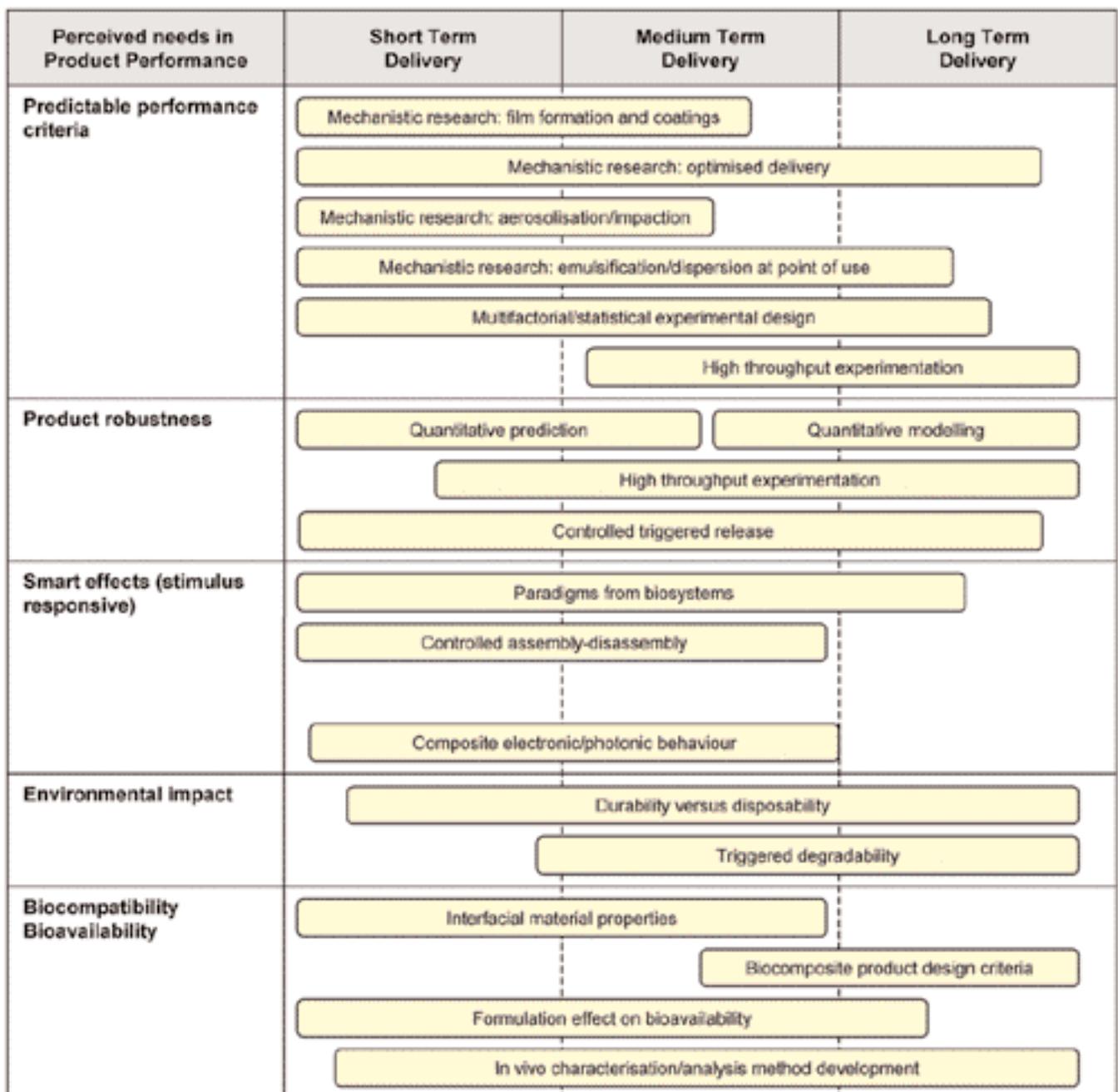
The availability of material to interact with biosystems is a complex combination of exposure route, active and passive partitioning effects, and metabolic and other biochemical activity, all of which can be mediated by the formulation vehicle of a product.

#### In vivo characterisation and analytical capability:

Many of the current techniques which give information on material, physical or chemical properties of materials or interfaces with colloid-domain spatial resolution require conditions which are not easily adapted for use with in vivo materials. Research to be able to adapt techniques to use on such systems, for example higher pressure versions of ESEM, or new approaches, for example proximal probe microscopy, will be key to develop these capabilities, without which a mechanistic understanding of the processes important to deliver the potential described above, will not be possible.

In summary, likely key areas of research activity to meet these identifiable needs are collated in Figure 6.

Figure 6: Summary of “Product Performance” Research Themes





## 3.5 Customer expectation

This area covers those aspects of consumer perceptions of products that are often critically important in their choice of purchase, but are often aspects of product design, performance and manufacture which are determined by criteria which are adjuncts to the primary purpose of the product.

By way of example, a face cream may be primarily there to moisturise the skin, but the tactile qualities of the cream during application may be the critical factor determining choice of one product over another. Similarly, the primary purpose of paint may be to provide protection and decoration of a wall, but a product based on water instead of a volatile organic solvent may be preferred on the basis of lower environmental impact or reduced consumer-perceived odour during use.

### 3.5.1 User safety

This has, of course, always been a primary design criterion for chemically based products. However, the increasing sophistication of our understanding of the way in which chemicals interact with people is likely to give much greater knowledge of the composition of products in the future. In addition, the genomics revolution is likely to provide a vast store of knowledge of variation in individual sensitivity to different compounds.

#### Predictive toxicology:

While major research in this field is outside the scope of the remit of IMPACT, there are a number of aspects of dermal and inhalation toxicology which are determined by interfacial phenomena. In particular, the ability to study, and then model, the surface interactions of products with biological tissue (skin, eye, lung) is a key target in developing predictive toxicology.

#### Bioavailability and biocompatibility:

On a fundamental level, formulation vehicles, for example typically rich in surfactants, may significantly alter the intrinsic availability of other components of a product.

In pharmaceuticals, this may be used to optimise the uptake of drugs to maximise the therapeutic ratio. In other cases, the right choice of co-formulants might reduce the exposure to potentially harmful components. For example, the formation of surface barriers in cases of accidental contact or reduction of aerosolisation so minimising inhalation exposure.

#### Real time, ambient analytical methods suitable for use in vivo:

There is increasing potential for step change capability in methods to detect physical and chemical properties of complex systems at high sensitivity and spatial resolution. Many of the current methods cannot be applied to biological tissue in vivo, and this limits the mechanistic understanding of biocompatibility and bioavailability. Improvements in this area of capability are already in sight and are likely to make enormous impact on our understanding, and hence on product design, in this field.

#### Smart effects and controlled delivery:

Enhanced selectivity of product delivery is likely also to be a key to ensuring safer products by delivering the appropriate amount of active chemical only to the desired target at the right time. Delivery vehicles of colloidal dimensions will be increasingly in demand. Diffusion release systems encompassing release times from seconds to years are likely to be needed. Triggered release will be needed in response to a variety of environmental factors, for example temperature, pH, ionic strength, as well as to specific molecular recognition.

Triggered release will be needed in response to a variety of environmental factors, for example temperature, pH, ionic strength, as well as to specific molecular recognition.

### Ubiquitous sensors:

Exposure testing at point of use is likely to require enhanced developments of colloidal domain components resulting in cheap, disposable sensors that can detect a variety of chemical and physical parameters.

### Hygiene:

Developments in growing and emerging economies are likely to be enormous drivers for economic growth in the next century. Products based on colloidal technology to provide cost-effective routes to clean, bacteria-free or virus-free water are likely to be in great demand. In both first world and developing world economies, there will be increasing demand for hygienic, self-cleaning surfaces by the use of cleaning products or “smart” surfaces.

### **3.5.2 Low environmental impact**

#### Recyclability:

The increasing desire to recycle requires significant development of routes to disassemble multicomponent systems. This may include colloid and interface science which can be directly applied to product disassembly, or the initial design of product to “build-in” triggerable disassembly at the “end of life”.

#### Design of products using low environmental impact components:

While there have already been significant developments in products using more benign components, for example reduced VOC coatings, there is likely to be even greater activity in this field. In addition, the increasing scarcity of key resources, and calculation of energy input as part of the environmental life cycle analysis of products, is likely to raise future challenges, particularly in developing new low energy routes for product manufacture, for example using low temperature, low shear and thermodynamically spontaneous transitions.

### Products to minimise use of scarce resources:

The knowledge base and products developed using colloid and interfacial technology are likely to be key in developing new products to minimise use of scarce resources. By way of example, water is seen as being a major limiting resource in the next 50 years, and products based on colloidal and coating systems will become increasingly important in maximising efficiency of its use.

For example, the use of interfacial monolayers to reduce evaporative losses from reservoirs, in situ coatings to minimise leakage from distribution pipework, and the development of hydrogel materials to reduce water demand in agriculture, may well provide step change in the efficiency of use of this resource.

### **3.5.3 Low cost/performance ratio**

It is no surprise that, due to the range of industry interests represented in this review, there is a spectrum of bearable costs for the products they produce.

#### High performance products and materials:

It is clear that, in certain market sectors, the very high intrinsic value of new products will allow exploitation of cutting edge technologies, for example the emerging potential of novel, truly nanoscale materials. In these fields, the research activities that are likely to produce new opportunities include self-assembly at molecular scale to create truly nanoscale architecture devices using both inorganic and organic materials as well as biomaterial hybrids, and templated or self-assembled systems that allow “smart” functionality. In this arena, a particular challenge arises in the task of building up nanoscale functional units into mesoscale and macroscale devices. This is an area where supra-molecular and mesoscopic scale ordering is particularly dependent on colloidal forces.



#### Cost efficiency via efficient component design:

There is however going to be increasingly downward price pressure on established technologies that will require new approaches to both design and manufacture of colloidal materials. Here, the efficiency of material use, for example specifically designed surface-active materials could provide step change potential in the underlying costs of traditional products if they can be tailored cost effectively. It is possible that the post-genomics biotechnology revolutions, for example proteomics and metabolomics, could provide low cost routes to generation of such tailored materials via fermentation routes.

#### Cost efficiency via process efficiency:

Additionally, the efficiency of purification processes, many aspects of which are heavily dependent on colloidal domain processes, is a key target to minimise raw material costs.

### 3.5.4 Personalised products

#### Multidisciplinary profiling:

Increasingly, higher value products are being developed to provide bespoke products to individual needs, for example, the use of genomic profiling to develop drugs or smart/adaptable delivery vehicles profiles that suit individual sensitivity and susceptibility to treatment. This can only be achieved by drawing together a wide variety of scientific disciplines, and the requirement will increase for complex, multidisciplinary research activity to develop these new platforms of technologies.

#### Cultural drivers:

In addition, cultural preferences of emerging major consumer markets is likely to drive innovative product concepts which will require new technologies like, for example, the preference for “dry” shampoos in Islamic populations.

#### Direct interaction with customer:

The ability to utilise the increasing power of the internet as a direct contact between consumer and manufacturer is likely to produce increasing opportunities and demand for custom-made, personalised products. These will be ‘delivered’ at a distributed manufacturing facility and delivered direct to the consumer or even, in a more futuristic scenario, “manufactured” via a formulation/dispensing unit in the home. This would suggest that there would have to be a greater ability to predict the product design and performance characteristics of “families” of related products.

Examples at a retail consumer level might include: health treatment, personal care products, hygiene products or home products, for example decorative coatings. At an industry consumer level, this might include just-in-time, made-to-measure raw or component materials delivery.

#### Point of use diagnostics and sensors:

It is likely that this degree of customisation will also require increasingly sophisticated, but cheap and easy-to-use sensor or diagnostic devices, to aid the selection criteria of the personalised product. Point-of-care health monitoring devices/diagnostic chips are already entering the market place, and in an increasingly sophisticated consumer population, the demand for this type of diagnostic/personalisation is very likely to increase.

Require increasingly sophisticated, but cheap and easy-to-use sensor or diagnostic devices.”

### **3.5.5 Understanding customer-product interactions**

#### **Psycho-sensory product design:**

An area related to the degree of personalisation described above is the psycho-sensory response of the customer to products, for example foods or personal care products. The psycho-physical basis of perceived product performance is generally recognised as a neglected area of product design by companies operating in these fields. Examples include, what rheological characteristics make skin creams feel “good”, what psycho-sensory stimuli are key for customers to feel that products are “clean”.

This is an area requiring complex multidisciplinary research, and while some of it appears to be peripheral to the remit of IMPACT Faraday Partnership, it is clear the surface and mechanical properties of the materials concerned are likely to be key in understanding these phenomena, and it is here that the research is core to IMPACT activity.

#### **Whole person modelling:**

The desired outcome would be “whole person modelling”, suitably validated by appropriate empirical information, which would allow for new product development, personalisation to different types of customer and minimisation or negation of future requirements for animal testing for toxicology/safety assessments.

In addition, there is an opportunity to develop some innovative science that would service a variety of industrial sectors including pharmaceuticals, personal care products, hygiene/cleaning products and food products.

In summary, likely key areas of research activity to meet these identifiable needs are collated in Figure 7.



Figure 7: Summary of "Customer Expectation" Research Themes

Perceived needs in Customer Expectation	Short Term Delivery	Medium Term Delivery	Long Term Delivery	
<b>User safety</b>			Predictive toxicology	
		Bioavailability and biocompatibility		
	Sub-micron, in vivo, analytical methods			
	Controlled delivery and smart systems			
			Ubiquitous sensors	
	Hygiene systems			
<b>Low environmental impact products</b>	Recyclability			
	Use of low impact components			
	Products designed to aid resource conservation			
<b>High performance/cost ratio</b>		Nanotechnology – high performance products		
	Efficient component design			
<b>Personalised products</b>	Multidisciplinary profiling			
	New product concepts from cultural drivers			
	Response to direct customer demand			
	Point of use diagnostics and sensors			
<b>Understand customer-product interactions</b>	Psycho-sensory understanding for product design			
			"Whole person modelling"	

## 4. RESEARCH STRATEGY

It is worth noting that most topics raised in the above themes call for multidisciplinary research skills. Significantly, a concern expressed by many participants in this exercise is the relative weakness of the UK in developing multidisciplinary academic programmes compared with other Western European countries and the USA. Five dominant research topics have been identified:

When analysing the data generated during the colloid science and technology road mapping process, five themes were dominant:

- Prediction Modelling
- Controlled Colloid Architecture
- Controlled and Triggered Release
- Measurement
- Biological Colloid Systems

“Themes call for multidisciplinary research skills.”

### 4.1 Prediction modelling

This topic came through strongly with three key areas identified – formulation, process and toxicological modelling.

#### 4.1.1 Formulation modelling

What happens if an ingredient is changed? Can the interactions in a formulation mix be modelled to predict, for example, shelf-life stability? It is doubtful that modelling alone will provide robust answers to these commonly asked questions, but a combination of modelling with High Throughput Experimentation/Screening could provide a

powerful tool in the armoury of the formulator.

There is good existing knowledge in the pharmaceutical, and paint and coatings sectors, and cost effective technology transfer to other sectors is a clear target.

#### 4.1.2 Process modelling

This would provide a powerful aid both for scale-up, and in the original design and development of the process to produce a particular material. Crucial to advances in this area is the development of robust monitoring processes, and the increased understanding of complex manufacturing processes through the use of a modular approach. Portability, flexibility and cost-efficiency of manufacturing will then become more easily achievable.

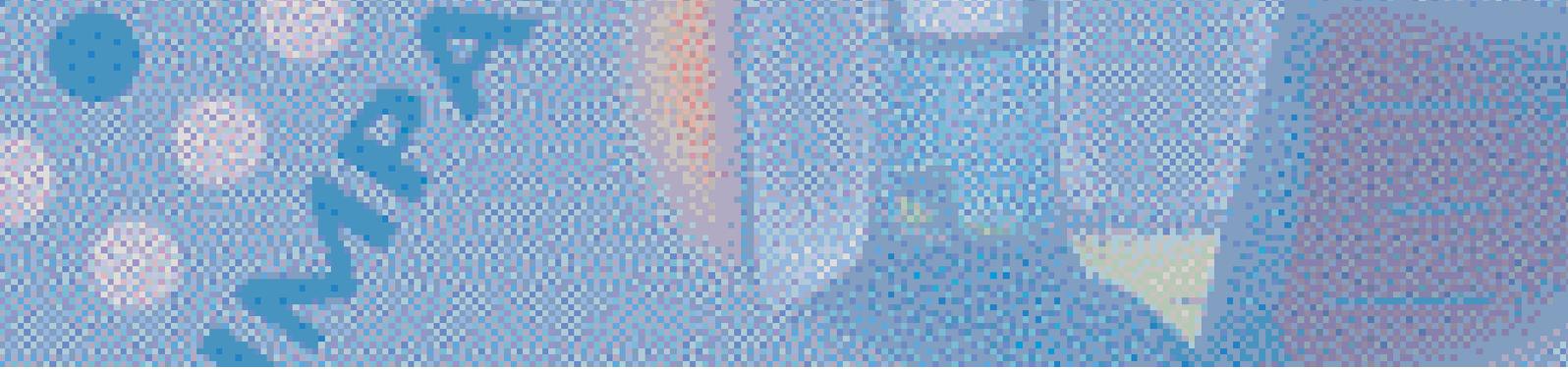
#### 4.1.3 Predictive toxicology

Predictive toxicology could be used to determine the impact of changing an ingredient in an established formulation through to the idealised concept of whole body modelling.

## 4.2 Controlled colloid architecture

A wide range of self-assembly processes was identified including controlled synthesis of nanoparticles, controlled crystal growth and production of complex multilayer films. An ambitious target might be the optimum catalyst – well ordered sized channels allowing access to all active sites (the perfect zeolite?).

“The most popular designer 3D structure that emerged from this consultation exercise was ‘reproducible synthesis, stabilisation and scale-up of nanoparticles.’”



The most popular designer 3D structure that emerged from this consultation exercise was 'reproducible synthesis, stabilisation and scale-up of nanoparticles'. The IMPACT-led Foresight LINK programme, ACORN<sup>2</sup>, aims to deliver against this objective. However, there is clearly room for increased investment in this emerging technology.

Although the main discussion focused on self-assembly of 3-D architecture, the concept of self-disassembly emerged, particularly with respect to recycling of complex materials, such as built-in 'triggerable' disassembly at the end of useful life.

## 4.3 Controlled and triggered release

This can be paraphrased as 'delivering the appropriate amount of active chemical at the right time to a specific target'. The ability to segregate potentially reactive components of multicomponent systems, allowing reaction/release on demand, is increasingly attractive. Development of appropriate triggered release systems is an important aspect. Many examples were highlighted, such as encapsulation (with release on demand) to reduce chemical degradation in storage and improved drug efficacy with reduced side effects. Triggers might respond to a variety of specific changes in environment, including pressure, temperature and pH.

### Colloid Science and Nanotechnology

There is much lively debate on the scope and potential of nanotechnology. Early products are emerging, but the true potential of this technology will take time to develop, and it is important to recognize that colloid and interface science is, and will continue to be, one of the major underpinning sciences required to deliver that potential. The importance of this science base falls into three broad categories:

a) The properties of nanostructured materials, which give rise to their unique properties, typically arise as domain size drops below a few hundred nanometers, where the surface properties dominate over bulk properties. The techniques for studying surface phenomena have primarily grown from the colloid and interface science community and are being further developed into real-time methods with sub-micron resolution. These techniques will be key to understanding and optimising "nano-devices".

b) There are many examples of novel effects deliverable from nanomaterials, but exploitation of these effects is critically dependent on the ability to develop

cost-effective manufacturing capability. Some nanomaterials, such as carbon nanotubes, are being produced in "industrial quantity", but for most of the prospective nanomaterials currently in research, there are significant hurdles to overcome to develop robust process engineering as for example in the effective manufacture of nanoparticles (see also the reference to ACORN Foresight LINK Programme in main text).

c) The novel properties of nanomaterials will often only be exploitable if there is a commercially viable route to creation of ordered structures of nanoscale sub-units. While "top-down" manufacture has been shown to be commercially viable, as in the silicon chip industry, the length scale limits of many manufacturing methods, for example in lithography processes, are now being reached. This has pointed towards "bottom-up" or self-assembly processes as a key target for achieving new materials based on nanoscale phenomena. This is an area of core competence in the colloid science arena, and is underpinned by knowledge from surfactant science, polymer composites, thin film manufacture and applications in biomimetic assembly processes.

<sup>2</sup> ACORN represents 'A Collaboration On Research into Nanoparticles' – [www.acorn-link.org](http://www.acorn-link.org)

An interesting development might be the smart agricultural sprayer. As with point-of-sale paint dispensers found in major DIY stores, could a mobile chemical factory be developed for crop management? Sensors would detect specific weeds triggering the release of the correct dose of appropriate herbicide formulation, resulting in more efficient use of ingredients with consequent reduction in environmental burden.

## 4.4 Measurement

Measurement emerged as the truly ubiquitous theme throughout the consultation process. From relatively simple technology transfer aspects of analytical services (that is, who can do what) through to real time analysis of complex formulation processes (for example, in-line/on-line analysis, and remote sensing of smart body implants).

“Measurement emerged as the truly ubiquitous theme throughout the consultation process.”

A major driver is the need to develop ‘cheap’ robust and reliable sensors. As noted under predictive modelling, development of high throughput, analytical techniques are a key requirement, and many of the triggered response systems will require specific sensor detection. Lab-on-a-chip development will continue, as will the need to miniaturise analytical systems. There is a clear need for higher resolution instrumentation for measuring and characterizing physico-chemical properties of nanoparticles and composite materials, biomaterials under in vivo conditions, and “real-world” materials, in-line or at-line, during manufacture.

The popularity of this theme is not surprising as it underpins virtually all topics raised.

## 4.5 Biological colloid systems

Bio-colloid systems are of growing importance, with one obvious example being the anticipated growth of enzyme catalysis. Highly specific transformations to novel ‘designer’ materials are a realistic target. Could ‘novel’ functionality be obtained via genetic modification of crop-based renewables? For example, production of designer functionality for triggering disassembly and thus aiding the environmental drive for recycling.

Advances in biomedical fields, for example, smart implants, composite structures and prosthetics, will require commensurate advances in biocompatibility to bridge the chemical-biological interface. IMPACT will seek to develop this theme further using a wider consultation of expertise, particularly with the biomedical sector.

Knowledge transfer between colloid and bioscience communities is also seen as a rich source of innovation. Examples include:

- a) colloid science knowledge of, for example, water structuring and interaction energies at macromolecular scale and at interfaces could be used to provide greater mechanistic understanding of biochemical and biological mass transport processes; and
- b) the ability of nature to utilise and control self-assembly in for example, biomembranes or supramolecular protein assembly, could provide new paradigms for the controlled synthesis of 3D colloidal structures.

“Knowledge transfer between colloid and bioscience communities is also seen as a rich source of innovation.”

## 4.6 Linking research themes and industry needs

Each research theme can be used to show how research activity can be correlated back to industry needs. This is summarised in Figure 8. The themes are broad and can be interpreted in a number of ways. By correlating with the industrial needs and drivers, we can identify where specific research concepts, novel ideas and opportunities arising from new science can be focused most effectively, to identify routes to commercial exploitation or allow the creation of new industrial capability.



Participants in IMPACT Faraday Partnership's innovative brainstorming session in Birmingham on 3rd October 2002

Figure 8: Framework of road map and research targeting

On the left is each key area where colloid science is a critical part of the process of adding value in the creation of products. In each of these areas, generic industrial needs are listed and an indication of the relative importance of each of the five major research themes identified in this research strategy is given using the following key:

- Research activity critical to delivery of step change capability
- Research activity useful for enabling elements of improved capability

Area	Industrial need	Prediction modelling	Colloid architecture	Controlled and triggered release	Measurement	Colloid and biological science
Ingredient base	Easily/reliable ingredient substitution	●		○	●	●
	Components' physical form	●	○		●	
	Product robustness (storage, manufacture, performance)	●	○	●	●	
Product manufacture	Process robustness and flexibility	●	○	●	●	
	Smart assembly of multicomponent products	○	●	○	○	●
	Distributed facilities	●		●	○	○
	Process efficiency	●	○	○	●	
Product design	Predictable product stability	●		●	●	○
	Link to manufacture process and product performance	●		○	○	
	More efficient products	○	●	●	●	
	Microparticle design	○	●	●	○	○
	Controlled 3D architecture	○	●		○	○
	Design link to product application process	●			○	
Product performance	Predictable performance criteria	●		○	●	●
	Performance robustness	●		●	●	
	Smart-effects (i.e. stimulus-responsive systems)	○	●	●	○	●
	Low environmental impact	○		●	●	●
	Biocompatibility or bioavailability	○	●	●	○	●
Customer expectation	User safety	○		●	○	●
	Low environmental impact	●		○	●	●
	High performance/cost ratio	○	●	●	○	●
	Personalised products	●	○	●	●	●
	Understand customer-product interactions	●		○	●	●

## 5. RECOMMENDATIONS

- **The report will be widely disseminated to the industrial and academic colloid and interface community.**

The objective will be to encourage discussion between the industrial and academic communities, and to generate collaborations with the aim of focusing research activity. Support for this focused, collaborative research will be sought from the UK Government and the EC.

- **The report will be used to focus current IMPACT research activity.**

It is the objective to map the current IMPACT (and ACORN) research activity, and compare against the Strategic Research Agenda identified here. Future IMPACT research will be focused on areas identified in this report as being important, but not yet receiving sufficient coverage.

- **Comparisons with Europe, the USA and Japan.**

It is intended to compare the findings in this report to activity at an international level. The main objective will not be for benchmarking, but to identify opportunities for collaboration.

- **Design of Technology/Knowledge brokering events.**

The information in the report will be used to identify specific opportunities for technology and knowledge transfer. IMPACT will organise small focused events, with previously identified 'sellers' and 'buyers' of technology and knowledge. Where appropriate these events will be held in collaboration with other Faraday Partnerships.

- **Sector specific technology audits and road maps.**

The report will be used as a starting point to generate technology road maps for specific sectors. The mechanism will be facilitated by IMPACT in collaboration with a single organisation or a consortium of organisations.

- **Development of relationships across the EU.**

The report will be used as the basis for collaboration with like organisations across the EU. It is expected that IMPACT will facilitate an application into the FP6 programme for a Network of Excellence within the next 6-12 months.

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## Principle authors

D K Rodham, D Parker, G Newbold, P Reynolds, T Gregory, and A Smith.

## Administrative support

C Richardson, K Snow, and M J Rendle (proof reading).

## Contributors

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## Attendees at Oct 3rd brainstorm

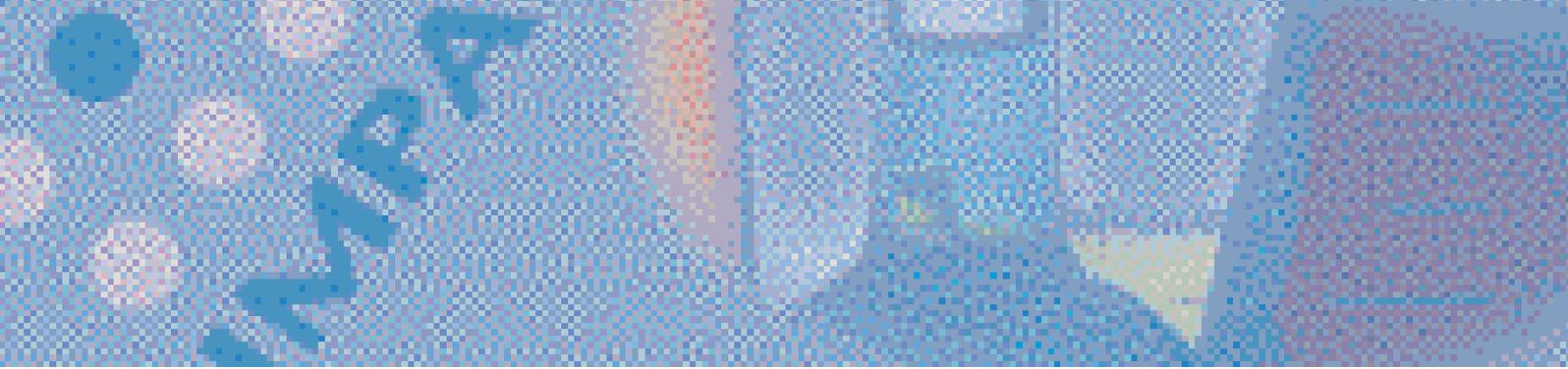
Prof Simon Biggs	University of Leeds	Dr Malcolm McKechnie	Reckitt Benckiser Healthcare Ltd
Prof Jon Binner	Loughborough University	Dr Paul Mills	DuPont Teijin Films UK Ltd
Mr Dave Cartwright	Cygnus Instruments Ltd	Dr Geoff Newbold	IMPACT Faraday
Dr Terry Corner	Muraspec	Dr David Parker	IMPACT Faraday
Dr James Dalton	Johnson Matthey plc	Dr Eric Paterson	Dow Agrosociences
Dr Steve Downing	ICI Paints	Dr Jonathan Phipps	Schlumberger Cambridge Research Ltd
Prof Michael Edwards	IMPACT Faraday	Dr Jon Preece	University of Birmingham
Mr Ray Elmitt	Crystal Game Plan	Prof Hamish Rankin	UMIST
Dr Stephen Elsbey	EPSRC	Dr Paul Reynolds	IMPACT Faraday
Dr Robert English	NEWI	Dr John Robb	Tioxide Europe Ltd
Dr Adrian Friedman	Syngenta	Dr David Rodham	IMPACT Faraday
Dr David Gardner	Pro-Bio Faraday	Dr Tim Ryan	Epigem Ltd
Dr Mike Garvey	IMPACT Faraday	Dr John Schofield	Avecia Ltd
Dr Adrian Geisow	Hewlett Packard Ltd	Prof Peter Schroeder	Quo-Tec Ltd
Dr Simon Gibbon	ICI	Dr Alan Shakesheff	QinetiQ Nanomaterials Ltd
Dr David Goddard	BNFL	Dr Martin Shenton	AG Fluoropolymers UK Ltd
Dr Richard Greenwood	University of Birmingham	Dr Alan Smith	IMPACT Faraday
Dr Trevor Gregory	IMPACT Faraday	Dr Ray Smith	New Game-Plan
Prof Keith Guy	IMPACT Faraday	Dr Simon Stebbing	Ineos Silicas Ltd
Dr Stan Higgins	James Robinson Ltd	Dr Ken Symes	CIBA Specialty Chemicals plc
Dr Andrew Howe	Kodak Ltd Research Laboratories	Dr David Tunnicliffe	BAE Systems
Dr Gary Leeke	University of Birmingham	Prof Dominic Tildesley	Unilever Research, Port Sunlight
Dr Stephen Lenon	Disperse Technologies	Dr Steven Walker	CCFRA
Prof Jian Lu	UMIST	Dr John Whittal	Crystal Faraday
Prof Paul Luckham	Imperial College	Dr Y Yin	Dytech Corporation Ltd
Dr Alan Mackie	Institute of Food Research		

## Attendees at Feb 5th brainstorm

Trevor Gregory	IMPACT Faraday
Jian Lu	UMIST
Ray Oliver	ICI
David Parker	IMPACT Faraday
Jon Phipps	Schlumberger Cambridge Research Ltd
Nick Quirke	Imperial College
David Rodham	IMPACT Faraday
Alan Smith	IMPACT Faraday
Dominic Tildesley	Unilever Research, Port Sunlight
Andy Ward	Rutherford Appleton Laboratory
Alistair Wilson	Waverley Consultancy
David York	Procter & Gamble

## Companies and academic groups visited by Technology Translators up to Feb 2003

A G Fluoropolymers UK Ltd	Johnson Matthey plc
Ahlstrom Corporation	King's College London
Alembic Products Ltd	Loughborough University
API Foils Ltd	North East Wales Institute of Higher Education (NEWI)
Avecia Ltd/Avecia Biocides/Avecia Biotechnology	Nottingham Trent University
Azko Nobel International Coatings Ltd	Nullifire Ltd
British Aerosol Manufacturers' Association	Organic Materials & Polymers University Innovation Centre
Building Research Establishment (BRE)	Oxford University, Department of Physical Chemistry
Cardiff University	Polyprep Research and Application
CCFRA	Queen's University, Belfast
Ciba Specialty Chemicals Plc	Reckitt Benckiser plc
CIRCE Ltd	Royal Society of Chemistry
Colormatrix Europe Ltd	Scottish Executive/Highlands & Islands Enterprise (HIE)
Columbian Chemicals Company	Siboro Ltd
CRYSTAL Faraday Partnership	Smith & Nephew Group Research Centre
Eco Solutions Ltd	Syngenta
Elementis Pigments	Teesside Chemical Initiative
Epigem Ltd	Tioxide Europe Ltd
EPSRC	Unilever Research, Port Sunlight
EuroCaps Ltd	University of Birmingham
Exeter Advanced Technologies (X-AT)	University of Cambridge
Fretwell Downing Education	University of Durham
Giltech Ltd	University of Hull
Gwent Electronic Materials Ltd (GEM)	University of Leeds
Heriot-Watt University	University of Nottingham
Hewlett Packard Ltd	University of the West of England
Huntsman Tioxide	University of York
Hyperlast Ltd	Veeco Instruments Inc
IChemE, Particle Technology Subject Group	White Rose Faraday Partnership
ICI plc	Winslow Adaptics Ltd
Institute of Food Research	WL Gore & Associates (UK) Ltd
International Food Policy Research Institute (IFPRI)	Yorkshire Forward
James Robinson Ltd	





IMPACT Faraday Partnership  
Science & Technology Centre, University of Reading  
Earley Gate, Whiteknights Road  
Reading, Berks, RG6 6BZ  
Tel: 0118 935 7000 Fax: 0118 926 7917

Web: [www.impactfp.org](http://www.impactfp.org)