Rational selection of thermoplastics

Materials selection is often made on the basis of experience, but sharper tools such as specialised software are needed when external drivers, for example the WEEE directive, force a change in design. Dr Patrick Coulter reports.

If it is choice you're looking for, then with around 50,000 different types of material on the market, thermoplastics could fit the bill.

This astounding range of properties arises as a result of the numerous combinations of base resins, fillers, and additives available to produce ready-to-form materials with precisely-tailored properties. The choice available means enormous scope for design and design optimisation in fast-moving and competitive areas such as the electronics, electrical, medical, and automotive industries.

We love choice, of course – until we have to make a decision! So which thermoplastic should you choose? How do you make that decision? Of the two tried and tested ways the first, and most widely applied in materials selection, is experience. It may be your own experience. What did I use last time? What materials am I familiar with? Or it may be the experience of others. Experience works, of course, but is also has its limitations.

Recently an industry colleague announced that he had made a better component using a material that no supplier would recommend for the application. This improvement was discovered by applying a rational property-based analysis to the problem. In doing so, he has given his firm a competitive edge, the source of which his competitors are probably not even aware of at this stage. This second approach is known as 'rational selection' of materials.

The rational method offers a means to both complement and go beyond experience in the selection of materials. It offers the prospect of discovering better, cheaper, faster ways of working.

On the face of it, rational materials selection looks easy. Following logic, a material's properties determine its relative suitability for a given application, and these properties can be measured and compared with those of other materials to decide on the best option. If only it were that simple! In general, actually implementing rational selection can mean meeting a series of nasty obstacles.

Obstacles to rational selection

Computer-based tools for materials selection have been available for over 20 years. From the product designer's perspective, they have delivered good information sources, but attempts at rational selection have, by and large, not achieved their promise. This is because the technical barriers to creating a working system have been formidable, and have taken a long time resolve. These obstacles include:

- Data collection – you can't select materials that you don't know about, so a working system needs technical data on tens of thousands of materials. To collect and computerise information from over 400 suppliers – and then keep it up to date – is a large and difficult task. There have been many attempts to build such collections, but the leader in terms of pure size and currency is a database developed by IDES Inc, which contains technical datasheets for around 50,000 materials.
- Comparability and standards – to compare materials on the basis of properties, the properties must be measured according to the same standards and test conditions. But this is rarely the case. So to create order out of chaos, CAMPUS (Computer aided material preselection with uniform standards) – a group of plastics producers including big names such as BASF, Bayer, Dow, DuPont, Degussa, and Ticona, was formed in the early 1990s. The CAMPUS group agreed to report materials properties according to a finite list of tightly-defined international (ISO) standards. This approach has met with success, and today's CAMPUS database contains 6,000 grades from 27 producers.
- Holes in the data – enter any materials database looking for a material set of say four constraints, and how many materials will it find? Of course it should find all materials that correlate with the input data, but in practice less than one quarter are typically returned. This is the 'holes in

the data' problem, which arises because testing is expensive and vendors do not run every test, or they run slightly different tests to each other. Around 15 years ago, Rapra Technology decided to tackle the problem and developed PLASCAMS, a database with no holes. To achieve this feat, the database contained several hundred generic materials that were compiled by experts from knowledge of thousands of actual vendor grades.

- Price – is a specific instance of the holes in the data problem. Price is mandatory for any rational selection exercise – how many real products are designed without minimising cost? However, you will be hard pressed to find a price per kg or lb on any material datasheet.
- Selection method – the selection method is defined by how the data is treated in order to reveal the optimal material for a design requirement. Unfortunately, two obvious methods do not work for real design problems – selection by property limits and by weightings The reasons why these do not work are clarified in the case study later.

A method that does work was published in 1991 by Mike Ashby (author of this month's 'Opinion', see p22) in his book *Materials Selection in Mechanical Design*, and was implemented in the educational software package Cambridge Engineering Selector (CES) from Granta Design Ltd. The method involves four main concepts – screening on constraints, ranking on objectives, the use of performance indices and Ashby bubble charts.

Function	Safe containment of electrical components Better thermal resistance than the usual PBT material
Objective	Minimise cost for specified stiffness
Constraints	
Tensile elongation	>2%
Heat deflection temperature (1.8 MPa)	>420˚F/230˚C
Tensile strength, break	> >15ksi/100MPa
Moisture resistant	<0.35% absorption at 24 hours
High resistivity	1e10^{15}μΩ.cm
Dimensional stability out of mould	< 0.01
Filler content	<40%
Injection mouldable	

Function-objective-constraint analysis – the first stage in the application of the optimal polymer selector (OPS)

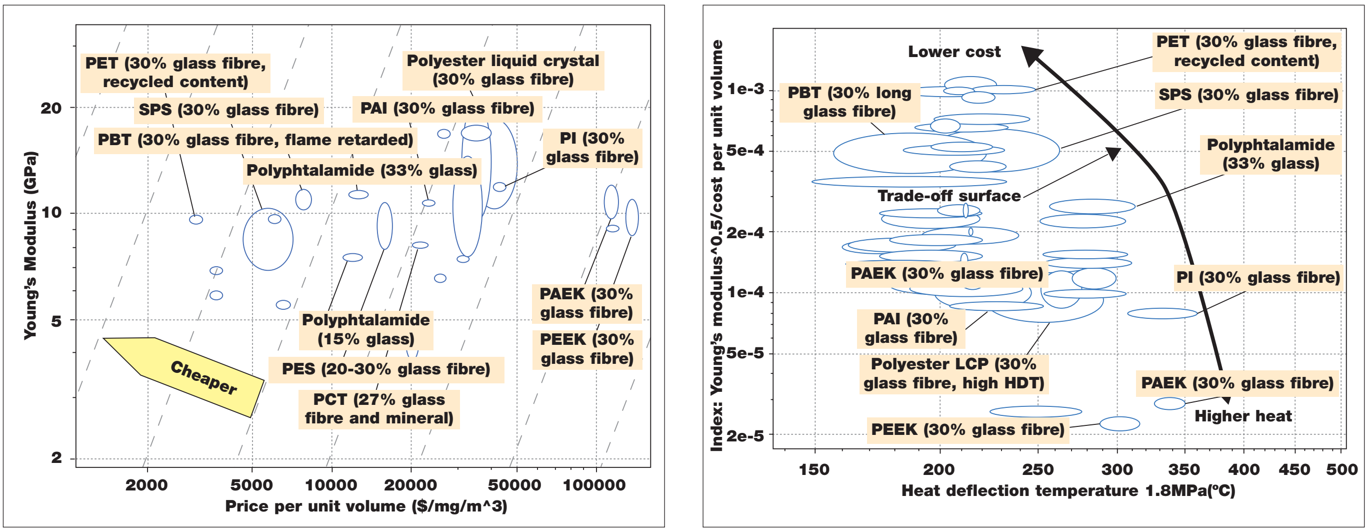
In addition to these obstacles, the choice is further complicated by the fact that material choice is intimately connected to the choice of manufacturing route and vice-versa. How can this be factored in? And how do you deal with further information that assists material decisions, such as handbooks and vendor websites? With so many hurdles, it is not surprising that real progress in rational selection has been a long time coming.

Optimal Polymer Selector

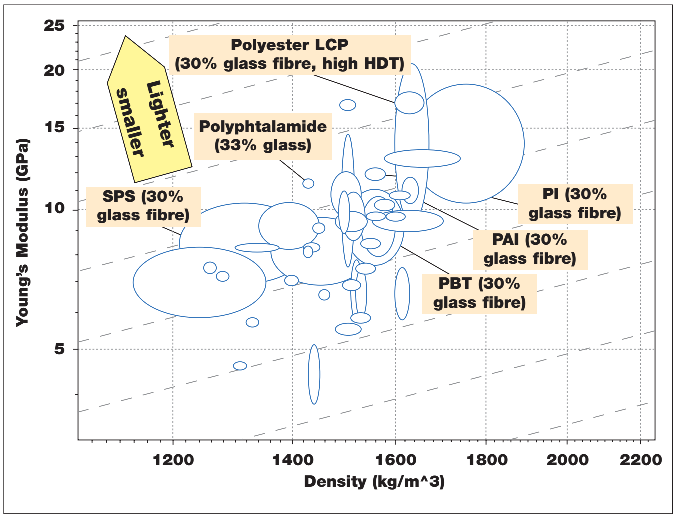
This summer Granta Design made the second major release of its CES Optimal Polymer Selector (OPS) package, making the bold claim that it is 'the most powerful plastics selection tool ever built'. Granta justifies this claim on the basis that the latest OPS overcomes all of the obstacles previously described, with all solutions combined into a single package.

Case study – choosing an electrical connector housing material

To illustrate OPS rational selection, consider the choice of a material for an electrical connector housing. Glass-filled polybutalene terephthalate (PBT) is a standard choice for this application. But what happens when an external factor changes the design requirements? One such driver of change is the Waste Electrical and Electronic Equipment (WEEE) directive, and in this case, lead-free solders may require higher temperatures for soldering, leading to the need for greater structural integrity of the plastic housing component.



Case study – choosing an electrical connector housing material. An Ashby bubble chart is plotted with price as the main criteria, left. Axes are on log scales with the bubble size representing the range of typical properties. The trade-off between cost and resistance to temperature is shown, right



Ashby bubble chart with low weight as the main criteria

The first step in the application of OPS is to perform a function-objective-constraint analysis, shown left. All eight constraints are straightforward material properties in this case, and the objective – the factor we wish to make as small as possible – is cost.

It can be concluded that the design is stiffness limited, and that the primary mode of loading is in bending rather than tension. From this, the correct performance index is rather unexpected – cost per unit volume over the square root of the stiffness. In terms of database material properties the index (M_1) is density (ρ) x price per unit mass (c_m)/ sqrt of modulus (E).

The results can be plotted as an Ashby bubble chart (opposite – below, left) based on the no-holes generic PolymerUniverse database. Recycled glass-filled PET is a cheaper option than PBT and glass-filled syndiotactic polystyrene (SPS) is also in consideration. The chart shows 24 further materials (out of an original 529) that meet the technical criteria, but are significantly more expensive per unit of bending stiffness.

Now for some 'what ifs'. A further chart (opposite – below, right) shows the trade-off between cost per unit of function and resistance to temperature. The best materials are always those close to the trade-off surface. So if PET, PBT and SPS materials fail due to heat, the next best choices are polyphthalamide materials, a few times more expensive, followed by polyimides, an order of magnitude more costly.

What if either miniaturisation or low weight take precedence over cost? Another material family, glass-filled liquid crystal polyesters, becomes the best choice (see left).

The list of possibilities could go on – what if resistance to motor fluids or acids or bases is needed? (OPS contains RAPRA's ChemRes ratings for this purpose). What if the connector must be transparent? Rational selection gives the designer the power to optimise with an authority only limited by the depth of the initial analysis.

Having now decided on, say, glass filled polyphthalamide, specific grades and suppliers can be chosen using either the CAMPUS or IDES databases. IDES has the advantage of size and CAMPUS the advantage of excellent comparability.

OPS identifies 118 glass-containing grades in IDES from eight alternative suppliers. These 118 grades can be narrowed down in OPS based on detailed requirements such as UL94 rating, weathering resistance, lubricity, or processing attributes such as flow.

Further information sources can be searched directly from OPS via Granta's MatData.Net service, for instance those of NPL, TWI, or ASM's Engineered Materials Handbook.

Large, rational steps

Huge strides have been made to make rational selection possible, and the benefits to come will affect everyone who designs with thermoplastics. So what is the next frontier? Arguably, it is the integration of rational selection in design with corporate processes – in particular to bridge the gap between the technical and commercial – in procurement, cost reduction, and preferred supply.

Optimum Polymer Selection access through Materials Information Service

One of the most important aspects of plastics component design is the choice of polymer to be used. The material chosen usually represents 40-60% of the cost of the manufactured item and consequently warrants special attention. Somewhat surprisingly, this is not always the case. Attention is certainly given to choosing the correct material, but the process is not informed by the latest experience and knowledge base. This is especially short-sighted as in an increasingly litigious business environment, the penalties for failure can be great.

To generalise, many UK converters would prefer the material choice to be made by the end-user, whereas continental European converters see this as their responsibility, since their process can alter the properties of the material in so many ways.

To carry out a relevant selection it is now increasingly important to incorporate the use of the latest relevant databases such as CAMPUS (Computer Aided Material Preselection with Uniform Standards), so that the choice of material can be justified in a technically competent fashion.

The Institute of Materials, Minerals and Mining's Materials Information Service (MIS) is becoming increasingly involved in these types of selection decisions, and its experience has shown that to do this properly it is critical that the design requirements are properly categorised, and following this, a comprehensive database is used for the selection process. This is where the latest Granta Design Cambridge Engineering Selector (CES) comes into its own. Once the OPS has 'spoken', then relevant MIS experience can be taken advantage of by the end-user or moulder.

Granta Design is a member of the Institute's Industrial Affiliate Scheme (IAS) and considerable experience in materials choice is now available through MIS using OPS – in the first instance to members of the IAS. The MIS team can also assist in making contact with the supplier base/qualification to establish the available specifications, and if necessary, help evaluate the material chosen.

Jan Czerski, Materials Information Service

Author details

Dr Patrick Coulter is Chief Operating Officer of Granta Design Ltd, Cambridge, UK. Tel: +44 (0)1223 518895. E-mail: patrick.coulter@grantadesign.com. For further information on the Cambridge Engineering Selector, visit www.grantadesign.com.