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Materials selection for optimal environmental impact in mechanical design

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Abstract

In engineering design, material selection is carried out in a number of ways. There are many factors affecting material choice for a particular application such as cost, weight and processability, but some of the most important are those of mechanical performance. Many methods exist for optimising parameter values in mechanical design allowing activities such as minimum weight design, design for minimisation of thermal distortion and minimum cost design. These considerations are important but in recent years environmental factors have played an increasing role in the selection of materials and technologies. The inclusion of realistically complex environmental criteria in the design process necessitates the development of methodologies and tools to assist designers. This paper looks at one particular method of material selection in mechanical design: material selection charts by Ashby, and shows how this methodology can be extended to take environmental factors into account. The method for calculating both air and water pollution indices is explained and it is shown how these values may be used to plot charts. By producing material selection charts, along the lines of Ashby's method, which deal with air or water pollution, mechanical design for optimal environmental impact may be structured and accelerated. The limitations of the charts presented in this paper are discussed. © 1998 Elsevier Science Ltd. All rights reserved.

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1. Materials selection for mechanical design

Materials properties and selection are very important areas and there are many publications and data sources available such as books by Ashby [1], Chong [2], Crane and Charles [3], ASM [4] and computer programmes such as PLASCMAS [5], CAMPUS [6] and Cambridge Materials Selector (CMS) amongst many others.

When selecting materials, designers and engineers have to take into account a large number of factors. These factors range from mechanical and electrical properties to corrosion resistance and surface finish. In

mechanical design it is the mechanical properties which are of greatest importance. There are a wide range of material properties which can be considered in mechanical design some of which are shown in Fig. 1.

The relative importance of each of these properties will be dependent on the application in question. It can be seen that different classes of materials exhibit specific mechanical properties. Metals tend to be of a high stiffness, strength and ductility while having a high density. Polymers are lower in density with generally lower strength and stiffness. Because properties are grouped in this way certain classes of materials tend to be suitable for particular applications.

There are of course exceptions to these general properties in most material groups. Alloys and composite materials may exhibit properties which are considerably different from those of their pure counterparts.

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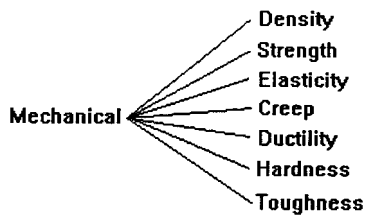


Fig. 1. Some material properties important in mechanical design.

Appropriate combinations of these properties will dictate the suitability of a material for a specific application. For example, values of density and Young's modulus or modulus of rigidity will be used to select materials which are light and stiff; density and strength will be used to select materials that are light and strong and so on. It is the ratio of these properties which will change for different applications. These ratios of properties are referred to by Ashby and Cebon [7] as material indices. Ashby goes on to define a material index as 'a grouping of mechanical properties which, if maximised, maximises some aspect of the performance of an engineering component'.

2. Material indices and design criteria and goals

When designers and engineers have decided on the important design criteria, the combination of parameters which best describes it (or needs to be optimised) may be derived as the material index. For example minimum weight design of stiff ties, beams, shafts, columns and plates relies on values of density and Young's modulus but in differing proportions.

The material index for minimum weight design of stiff ties is E/ρ ; the material index for minimum weight design of stiff beams, shaft and columns will be based on $E^{1/2}/\rho$ for bending loads with the shape of the section specified.

The design of stiff plates loaded in bending will rely on a material index of $E^{1/3}/\rho$; where E = Young's modulus and ρ = density. In most cases it is the maximisation of these indices which is the design goal. Other combinations of properties may be used to optimise materials selection based on such criteria as, strength-limited design, vibration-limited design and even cost-limited design.

Design is dictated by a number of factors, but they can be classified very simply into two areas:

1. Objectives; and
2. Constraints.

Objectives are aims or targets to be achieved by the designer such as reducing mass or size, or energy content. The degree to which these objectives are

achieved will be dictated by the constraints. Constraints can be related to main factors such as cost or mechanical function. If the constraints are related to mechanical function then parameters such as strength or stiffness become important. It is these objectives and constraints which may be used to decide on which material indices need to be used.

Ashby and Cebon [7] identify three main steps in compiling material indices:

1. Function;
2. Objective; and
3. Constraint.

These three stages can be developed in more details to what Ashby and Cebon refer to as a 'recipe' for deriving material indices shown in Table 1.

Many examples of these material indices and their applications are given in *A Compilation of Material Indices* by Ashby and Cebon.

The properties used in the material indices will usually be grouped in ranges by material types. As this is the case it is possible to plot charts to give a graphical representation of material groups in terms of properties. By doing this the appropriate material indices may also be plotted on the charts and used to select groups of materials which meet the requirements of the objectives and constraints.

3. Ashby's material selection charts

According to Ashby [8] 'The Materials Charts are most effectively used by plotting performance indices onto them, isolating a subset of materials which opti-

Table 1
Deriving material indices [7]

Stage	Requirement
a	Identify the aspect of PERFORMANCE P (mass energy content, etc.) to be maximised or minimised
b	Develop an EQUATION for P (<i>the objective function</i>)
c	Identify the FREE (unspecified) VARIABLES
d	Identify the CONSTRAINTS; rank them in order of importance
e	Develop EQUATIONS for the constraints (no yield; no buckling, etc.)
f	SUBSTITUTE for the free variables from the constraints into the objective function
g	GROUP THE VARIABLES into three groups: functional requirements, F , geometry, G , and material properties, M (and possibly shape, S) thus performance $P \leq f[F, G, M, (S)]$
h	Read off the performance index, M , to be maximised

mally meet design goals'. Ashby's work has given us the material selection chart in the form shown below. Designers may choose from over 18 material selection charts and process selection charts which cover most areas of mechanical design. Plotting design requirements onto them and using a number of charts sequentially allows the simultaneous consideration of several design goals. Fig. 2 shows Ashby's Modulus–Density chart which can be used for the design of stiff lightweight components.

As can be seen the chart encompasses a large range of engineering materials and allows the designer to use the appropriate indices as design guidelines. The guidelines are plotted on the chart as lines of constant slope, the value of the slope depending on the particular application.

For example the design guideline slope for beams in bending of material index $E^{1/2}/\rho$ will have a gradient of 2. As the lines are moved towards the top left hand side of the chart the constant C increases. Therefore the materials with the best stiffness to weight ratio lie towards the upper left hand corner of the chart.

Further design constraints may be dealt with by successive use of different charts. For example a cost constraint may be added to the design. A further materials selection chart which considers unit cost would be the next filter in the selection process. Examples of these multiple stage selections are given in Ashby and Cebon's publications and guides.

4. Ashby's materials selection charts and the environment

Ashby's work deals with many material properties that are classed as environmental. In most cases these are properties concerning the reaction of the material to certain environmental conditions such as heat, moisture, chemicals and so on.

When environmental concerns in materials selection are taken as meaning the effect the material has on the environment, e.g. emissions, waste, etc., only one small, though very important, area is covered by Ashby's work; energy content.

In Ashby's method energy content may be used just as any other material property, in composing material indices for different applications. By plotting a chart of energy content per unit volume of material against failure strength on a chart, materials for strong, energy-efficient ties may be selected. Fig. 3 shows an example of one of Ashby's energy content material selection charts.

In terms of environmental design this particular chart can be very useful. One of the main aims of environmental design may be to reduce the energy requirement of a product or system. In some cases the energy content of the material is by far the greatest contributor to the overall energy requirement of a product or system. Using this chart allows the selection of energy-

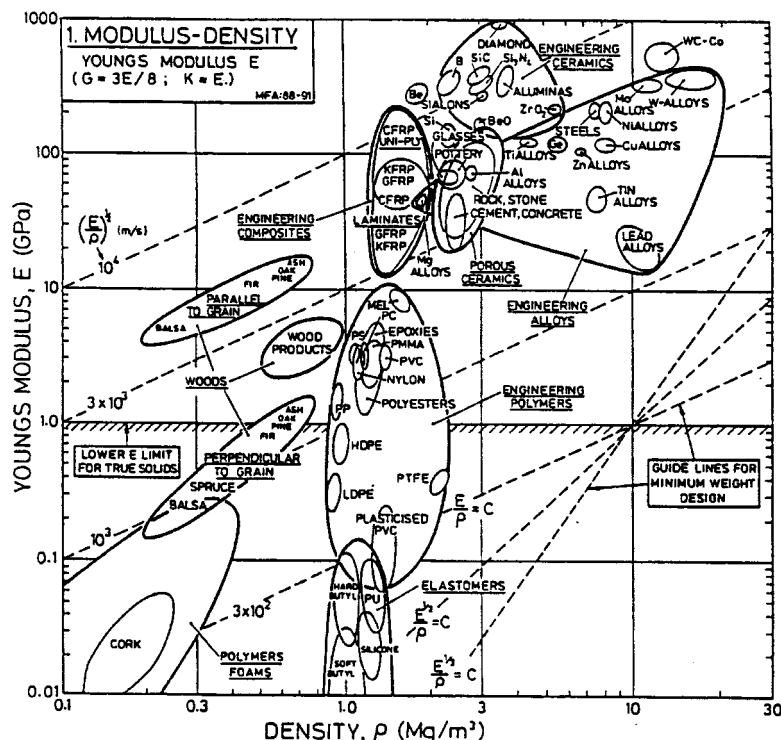


Fig. 2. Ashby's modulus–density materials selection chart.

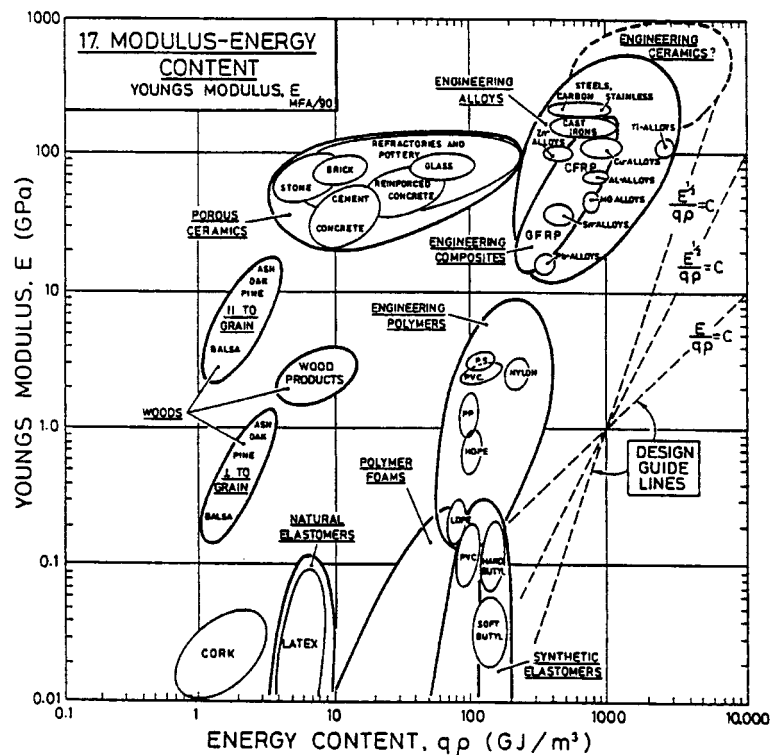


Fig. 3. Ashby's modulus-energy content materials selection chart.

efficient materials for specific mechanical requirements.

5. Environmentally-based materials selection in mechanical design

In the past energy use and content has been one of the few quantifiable aspects of environmental performance and could therefore be used in materials selection exercises. However, with increased environmental awareness in all sectors of industry, environmental data on the effect of material production and processing is becoming more readily available. Although quantifying the amount of a single pollutant, such as for example CO_2 , emitted through production of a material, is a complex task, it is relatively simple when compared to the problems which can arise when trying to assess the overall environmental effect.

Most designers and engineers, when designing for the environment, want to assess the overall environmental effect of both production and processing of a single material or a combination of materials. The production of a single material can result in over 100 inputs and outputs, emissions and waste products. Plotting charts for each of these emissions would be very time consuming and more importantly, would overwhelm the designer with massive amounts of data. By utilising concisely presented agglomeration schemes

such as MAC and O.v.D, however, normalised overall environmental effects of materials may be calculated and plotted on the appropriate materials selection charts.

6. Environmental data for material selection

In order to generate environmentally-oriented materials selection charts, environmental indices need to be calculated. Other materials selection charts contain discreet data, giving actual values of properties such as tensile strength, density or energy content per unit volume. In environmental terms, discreet data is easily produced for single emissions, but not for a combination of different emissions. For example we can say that production of 1 kg of ABS polymer will result in a total emission of 1.98 kg of carbon dioxide gas (on average). If we then go on to consider other emissions as the result of this production, we see that there are over 10 separate emissions to atmosphere and almost as many to water. This could cause major difficulties in representing this as discreet overall data. Although in some cases providing individual representations such as amount of CO_2 or SO_2 will be necessary, figures aggregating airborne and waterborne emissions are needed to reduce the amount of data being processed.

In order to compare emissions on an agglomerated basis we must be able to say which emissions are more

'serious' than others and attach a weighting as necessary. In certain cases, for example, we may need to compare the seriousness of the emission of 1 kg of CO and the emission of 1.2 kg of NO₂. This may be done effectively using MAC values and O.v.D norms. MAC values are '...the definition of acceptable levels in working conditions by the Dutch Labour Inspection' [9] and are used for airborne emissions. O.v.D norms are '...Dutch norms for maximum levels at the inlet of drinking water into purification plants' [9]. In this work we are using the Dutch definitions but other documented legislative data may be used as it may vary from country-to-country. If we define polluted air or water as air or water which is lost to human consumption without first needing treatment, then the MAC and O.v.D values offer comprehensive data for calculation.

In our sample case of comparing CO to NO₂ we can decide which is the worst case as follows:

MAC value of CO = 29 mg/m³;
 MAC value of NO₂ = 4 mg/m³;
 'Seriousness' of emission =

$\frac{\text{Actual Emission Value (mg)}}{\text{MAC Value (mg/m}^3\text{)}}$; for CO =

$$\frac{1\,000\,000}{29} = 34\,482.76 \text{ (m}^3\text{)};$$

$$\text{for NO}_2 = \frac{1\,200\,000}{4} = 300\,000 \text{ (m}^3\text{)}.$$

Therefore it can be seen in this case that the emission of CO will pollute 34 482.76 m³ of air and the emission of NO₂ will pollute 300 000 m³ of air. A problem arises here in that although we can calculate the theoretical

amount of air which is polluted by an emission we cannot say, with certainty, into what volume of air this polluted air is being released and how polluted that air is already. This system of calculation is therefore more useful for comparison or qualitative assessment than in absolute terms. To this end we can use the values as indices; ignoring the units. In this case the total air pollution index of both the emissions above will be 334 482.76 (300 000 + 34 482.76).

Calculations for emissions to water are carried out in the same way using O.v.D values in place of MAC values. Any number of these emissions may be added together to give an overall index to a system. The lower the value of the indices the less polluting the system. Theoretically, as the indices have no units, the air and water indices could be added together to give an overall index, but an exchange rate between air and water would be required and at this time there is no such rate.

Valuable data can also be lost by grouping them together so in order that informed decisions can be made by designers and engineers the air and water indices are best left separate.

Table 2 shows an example of what is an apparently simple system, the manufacture of 1 kg of HDPE. With 13 different emissions to air and 11 to water the system could become very complex when trying to express its overall effect on the environment without the use of an aggregation system.

By dividing each separate emission by its weighting factor and summing the results from emissions to like mediums we can arrive at an overall Air Pollution Index (API) and an overall Water Pollution Index (WPI) for the material. API and WPI indices can be calculated for any system whose emissions are known.

It should be noted that the effect of CO₂ emissions

Table 2
Emissions due to the manufacture of 1 kg of HDPE

Atmospheric emission	(mg)	MAC (mg/m ³)	Waterborne emission	(mg)	O.v.D (mg/m ³)
Acidic ions	100	4	BOD	100	7000
Ammonium ions	10	10	COD	200	30 000
Carbon dioxide	9.4 × 10 ⁵	–	Dissolved	20	50 000
Carbon monoxide	600	29	Organics	500	50 000
Chloride ions	800	3	Dissolved solids	150	0.2
Dust	2 × 10 ³	10	Hydrocarbons	300	500
Hydrocarbons	50	500	Metals	10	5000
Hydrogen chloride	1	2.5	Nitrates	30	0.2
Hydrogen fluoride	1	0.1	Oil	5	50 000
Metals	10 × 10 ³	4	Other nitrogen	1	200
Nitrogen oxides	5	1	Phosphates	200	50 000
Other organics	6 × 10 ³	5			
Sulphur oxides					
Total API		4277.5	Total WPI		915

Table 3
Comparison of pollution indices of HDPE and PET

	API	WPI
HDPE	4277.5	915
PET	20646	2106.3

is not included in these calculations as an MAC value is not yet available.

If we compare HDPE to another similar polymer such as PET (Table 3), we see the following in terms of pollution indices.

The much higher WPI value of the PET results from a 10-fold increase in the amount of oil released to water, which has a very low O.v.D value. What seem very similar materials in mechanical terms perform very differently in environmental terms.

The system of aggregation presented here is not the only way in which to group environmental effects. Other agglomeration systems are currently in use with the Eco-Indicators method which presents results with eco-points being the most popular. This system is used in the SimaPro, Eco-It and Eco-Scan software-based design tools. Rather than presenting water pollution and air pollution as separate entities the system presents a single figure for environmental impact in terms of eco-points. This type of presentation does have advantages of simplicity but there are questions which have to be asked about presenting complex environmental effects as a single figure. Valuable detail can be lost and over simplifications made when choosing materials on the basis of this information.

7. Environmentally-based material indices

If we are to plot environmentally-based materials selection charts we need environmentally-based design criteria and material indices. If we look at Ashby's energy content materials selection chart we can see that examples of material indices are:

$$\begin{aligned} E/q\rho & \text{ (minimum energy design of stiff ties); and} \\ E^{1/2}/q\rho & \text{ (minimum energy design of stiff beams shaft} \\ & \text{and columns).} \end{aligned}$$

Energy content is directly related to the mass of a material, and when multiplied by density it becomes a function of volume in joules per metre cubed. API and WPI values are also related directly to the mass of the material as all emissions data is in milligrams per kilogram of material produced. Therefore in multiplying density by API or WPI they also become a function of volume and can be plotted on materials selection charts in the same way as energy.

By considering the environmental factors in question we can produce the following material indices:

$$\begin{aligned} E/API\rho & = C \text{ (minimum air pollution design of} \\ & \text{stiff ties);} \\ E/WPI\rho & = C \text{ (Minimum water pollution design of} \\ & \text{stiff ties); and} \\ E/X\rho & = C, \text{ where } X = \text{specific emission (mini-} \\ & \text{mum emission design of stiff ties).} \end{aligned}$$

Design criteria for beams, shafts and plates will follow the same lines as above using $E^{1/2}$, etc. Criteria for design of strong and brittle components will follow the same lines as follows:

$$\begin{aligned} \sigma_f/API\rho & = C \text{ (minimum air pollution design of} \\ & \text{strong ties);} \\ \sigma_f^{2/3}/WPI\rho & = C \text{ (minimum water pollution design} \\ & \text{of strong beams and shafts);} \\ K_{Ic}^{4/3}/API\rho & = C \text{ (minimum air pollution design of} \\ & \text{brittle ties); and} \\ K_{Ic}^{2/3}/WPI\rho & = C \text{ (minimum water pollution design} \\ & \text{of brittle plates).} \end{aligned}$$

As can be seen most of the standard design criteria guidelines may be adapted to take environmental concerns into account and typically air and water could be used sequentially to select materials.

Now that we have 'pollution' or 'environmental' indices for different materials we can plot materials selection charts in terms of environmental concerns, giving engineers and designers easy to use comprehensive data for considering environmental design criteria. These charts will be plotted along the same lines as Ashby's energy content charts.

8. Environmental material selection charts

By using the same methods as Ashby and plotting environmental properties against mechanical properties a range of environmentally conscious material selection charts may be developed. Figs. 4–6 show three such charts.

Fig. 4 shows an 'emission-specific materials selection chart'. The x axis plots values of the amount of a particular pollutant released per unit volume of a material produced multiplied by density (in this case $\text{NO}_x \times \rho$), while the y axis plots the mechanical properties of the materials (in this case Young's modulus). This particular chart will allow engineers and designers to choose materials for a range of mechanical operations in which the emission of NO_x gas is optimised or reduced to a minimum.

Fig. 5 shows a 'total air pollution materials selection chart'. In this case the x axis plots the overall API

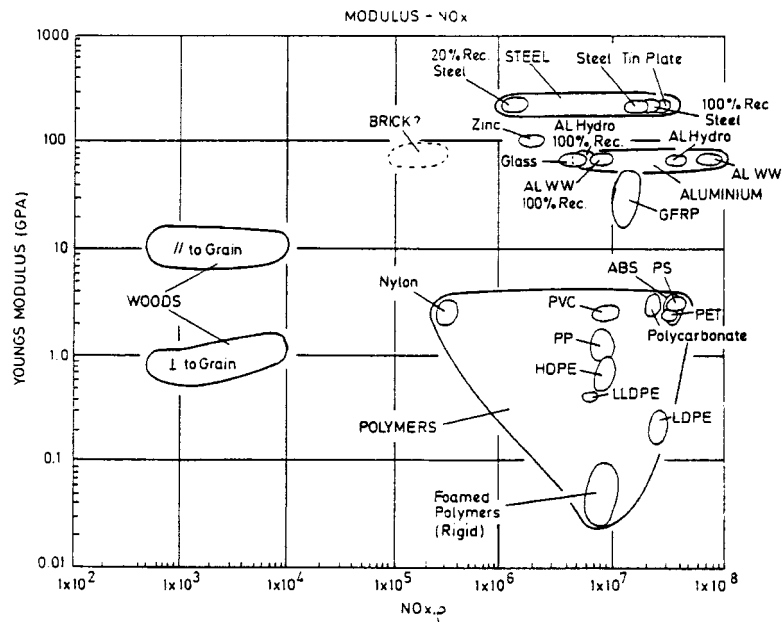


Fig. 4. Young's modulus- NO_x emissions materials selection chart.

values per unit volume of a material produced multiplied by density and, again, the y axis plots the mechanical property. This chart may be used to select materials which will fulfil mechanical requirements while reducing air pollution, as a result of material production, to a minimum.

Fig. 6 is another materials selection chart, this time covering overall WPI and strength. This chart is plotted and used in the same way as the others and allows the design of strong minimum water polluting components.

The design criteria guidelines plotted on these graphs are those discussed earlier. However, in the case of

environmental design determining a value for the constant C may be difficult. As design for the environment is a relatively new concern optimal values for C have not been calculated. As with other design criteria the higher the value of C the better the material is for the specified application. Design for the environment is set to become a very important part of mechanical design and as it becomes more common place the constant values for design criteria will develop.

At this stage designers should consider the overall range of API and WPI values for all the materials on the charts and make decisions based on relative com-

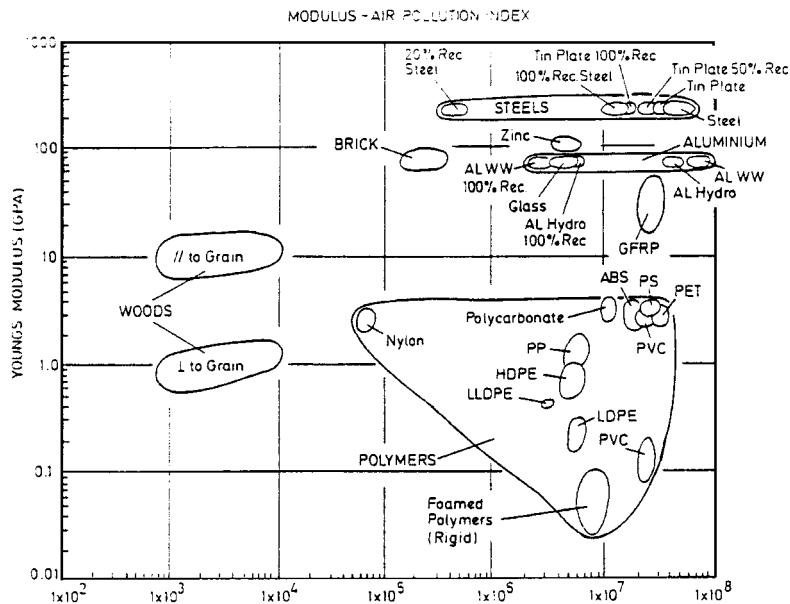


Fig. 5. Young's modulus-air pollution index materials selection chart.

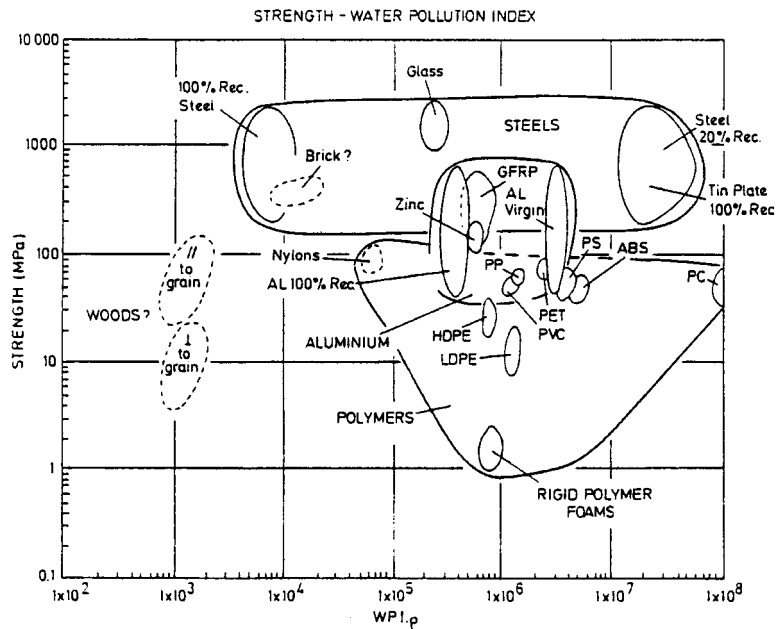


Fig. 6. Strength–water pollution index materials selection chart.

parison. The materials close to the bottom right hand corner of the charts will offer the worst environmental/mechanical performance with those at the top left hand side of the charts offering the best.

If a particular material is already in use for a specified application the charts will be useful in optimising material choice. A value of *C* may be calculated for the material which is already used and using the charts materials with a higher value of *C* may be selected.

9. Example — materials selection for drinks containers

The following example is carried out using the Cambridge Materials Selector (CMS) software package, including the environmental materials selection charts at the appropriate stage. Figs. 7 and 9 are direct outputs

of the CMS software. It uses the relatively simple example of a drinks container in order to illustrate the principle of the method.

Drinks containers come in a number of shapes and sizes but the most common is the standard cylindrical shape bottle. In this example we want to consider a container for fizzy drinks which can be approximated to a pressure vessel. As the walls of the vessel are thin compared to the overall dimensions we can approximate the bottle to a thin cylinder. In this case the cylinder is loaded in plane stress.

Table 4 summarises one possible design specification. The objectives include minimising water pollution arising from manufacture and also reducing the weight of the container. Because of the function of the container packaging, a considerable amount of its environmental impact will result from transportation. Reduc-

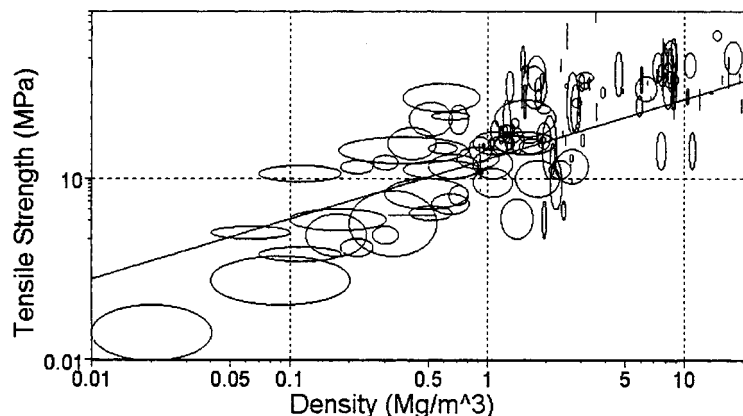


Fig. 7. Strength vs. density materials selection chart.

Table 4
Design specification for 'green' drinks containers

Function	Bottle: cylinder — plane stress
Objective	Minimise the mass of the bottle Minimise the water pollution resulting from manufacture
Constraints	1. Must be sufficiently strong 2. Must be adequately tough ($G_{ic} > 0.04 \text{ MPa}/\text{m}^{1/2}$) 3. Material must be cheap ($C_m < \text{£}1.2/\text{kg}$) 4. Material must be in the top 50% of all materials in terms of WPI emissions

ing the weight of the container will help reduce the impact in the distribution phase.

Stage 1 is the selection of materials suitable in terms of strength and density. As the container is being loaded in plane stress the parameter to be maximised is:

$$\frac{\sigma_f}{\rho}$$

Where σ_f is the strength of the material and ρ is the density.

A chart of strength vs. density is plotted and a line of slope 1 used to select materials (see Fig. 7). The second stage is to minimise the water pollution resulting from

manufacture of the material. In this case the relationship to be maximised is:

$$\frac{\sigma_f}{\text{WPI} \rho}$$

Where WPI is the water pollution index of the material.

Another chart is plotted, in this case of strength vs. $\text{WPI} \times \text{density}$. Once again a line of slope 1 is used to select suitable materials. This is shown in Fig. 8.

The final stage is the selection of materials within the limits of toughness and price. Fig. 9 shows this chart.

The full materials selection results are too lengthy to present in this paper. In this case the materials which passed all selection stages and thus can be deemed suitable materials for use in 'green' drinks containers can be summarised as (in order of mechanical/environmental performance):

- aluminium (preferably recycled);
- HDPE;
- PET;
- polypropylene;
- PVC (rigid);
- soda glass;
- steel (recycled); and
- zinc.

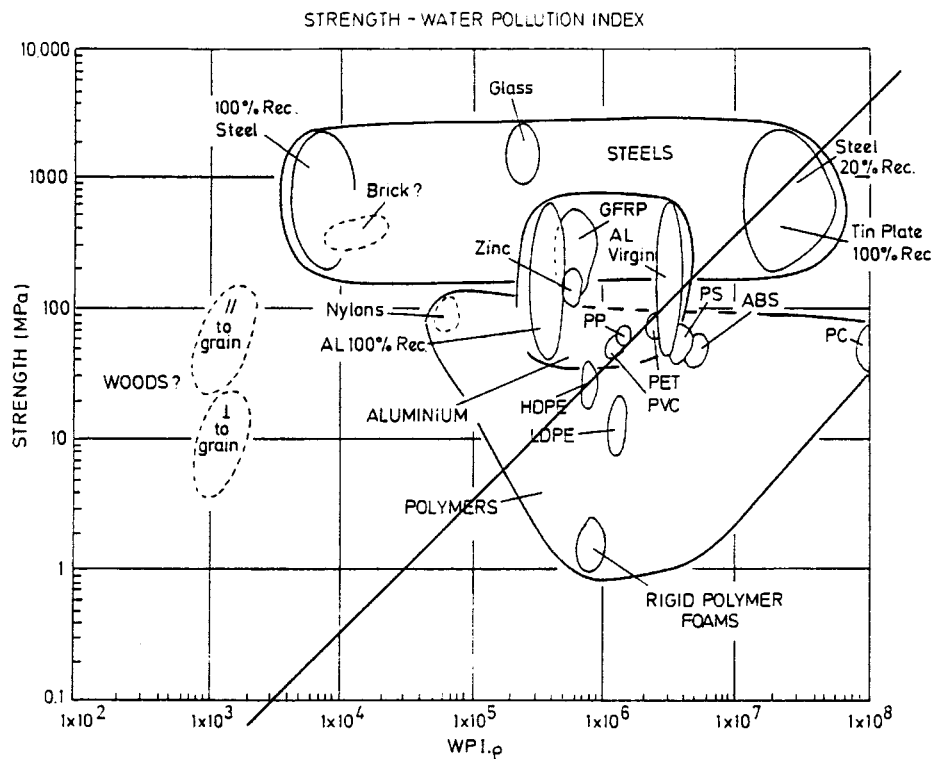


Fig. 8. Strength vs. WPI density materials selection chart.

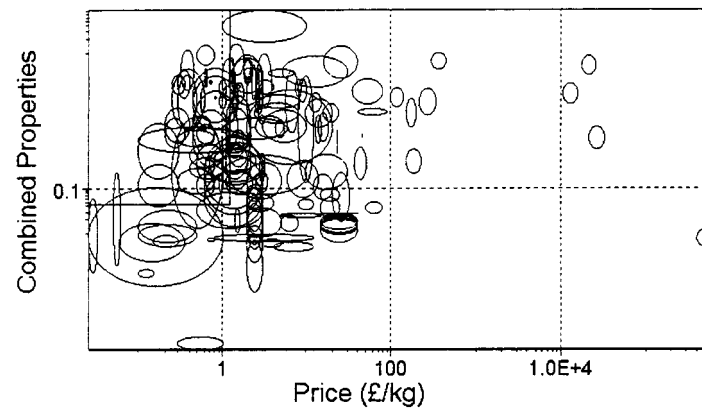


Fig. 9. Toughness vs. price materials selection chart.

10. Discussion of drinks container example

In this example the environmental data was only available for approx. 20 materials. Fortunately many of the materials for which data was available were suitable for the required application and so the final list of materials is sufficiently large to allow the designer a realistic number of possibilities. Most of the materials that are selected are in everyday use in this type of application. However, in this case we need to think about other parameters such as manufacturability and also permeability to carbon dioxide (for fizzy drinks). Glass, aluminium, steel and PET are all suitable for fizzy drinks and can be manufactured into containers relatively easily. PVC, polypropylene and HDPE are not suitable for use in fizzy drinks applications but are used for packaging liquids such as milk and orange juice. These materials can also be easily manufactured using injection moulding. In these applications less strength is required due to the lack of pressure loading on the container. Once again the metals selected are better environmentally if recycled but in this case the virgin materials also fall within the constraints of the design specification. Wood is a possible option but data is not available for the environmental selection stage. Also processing would probably rule out this material as there would be a lot of waste material generated through machining.

11. Limitations of charts and future work

The environmental materials selection charts presented in this chapter have a number of limitations and it is important that these limitations are understood in order that the charts may be used properly.

The emissions data for the materials in the charts is taken from a number of different sources: Boustead [10], Steinhage and Dam Van [11] and Habersatter and Widmer [12] amongst others. The data contained with these studies are averages of many different practices.

It should be understood therefore that the data these charts present may not be representative of particular operations used to produce the specific materials. The data is, however, an average of extensive studies carried out upon a large number of industrial operations and can therefore be used as a guideline.

None of the overall air pollution indices include the effect of carbon dioxide gas. There is, at this time, no accepted way of defining the MAC value of CO₂.

The number of materials in these charts is limited. The overall environmentally relevant inputs and outputs of a system are calculated using life-cycle analysis. LCA studies are very long and complicated operations and as it is a relatively new science not all materials have been the subject of such studies. The material groups contained within the charts presented in this chapter are, however, among the more commonly used materials in engineering design.

As LCA studies become more common place and the data will become more accurate, more emissions will be identified and more materials will be able to be added to the charts, making them more comprehensive and more useful. The use of the Eco-Indicators methods mentioned earlier in this paper is now becoming much more commonplace and data is available for a large number of materials. Aside from the problems of quantifying environmental impact with a single figure use of this system would allow much more comprehensive materials selection charts.

By using the method presented in this work environmental concerns may also be mapped onto process selection charts and extend Ashby's work further still. Charts such as surface finish vs. API may be plotted allowing engineers and designers to select processes which also optimise pollution.

12. Conclusions

With the problem of environmental pollution becoming more and more serious engineers and designers

must begin to take account of the effects that their design decisions have on the eco-systems around us. Unfortunately the integration of environmental concerns into the design process threaten to complicate it further still. In order that this does not happen there is a need for tools to support designers and help them to achieve their environmental goals. Rather than attempting to develop new design methods and aids, the adaptation of existing methods may afford the best opportunities. Ashby's materials and process selection charts are a tried and tested materials selection method. In the field of mechanical design these charts are a simple and quick way of assessing whether a material is suitable for the case in hand. By taking these charts and extending their range to include environmental concerns, designers may consider them in exactly the same way they consider other material and process properties.

Although these charts have a number of limitations they are still an important addition to a designers tool kit. Limited environmental information is better than none at all and by developing such methods and approaches now when environmental information becomes readily available the tools with which to manipulate this data will already be in place. It is the type of method or tool favoured by Billet [13] as it can be easily and be readily used by designers who need not have extensive knowledge of factors affecting design and the environment. Environmentally conscious material selection charts structure and accelerate the environmental impact assessment of design decisions and

readily integrate them into existing mechanical design procedures.

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