Process simulation for waste management

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SYNOPSIS A critical assessment of available options for waste separation, recycling and energy recovery is an essential strategic step in formulating an economic and technically viable waste management policy. The underpinning data for each assessment includes the provision of characterisations of the waste and quantification of its response to separation (either centrally or at source). These data are however difficult and expensive to obtain (at least conventionally through survey and practical work). They can alternatively be derived, to the necessary resolution but very much more cost-effectively, using predictive modelling methods. (i) Specific waste characterisation data can be predicted from alternative data sets, once these are formulated as functions of measurable objective criteria. (ii) Generic separation models based on measured performance data can be developed to provide the required catalogue of separation responses, for the whole spectrum of separation regimes. This paper describes the integrated role of 'characterisation models' and 'process' models. This is presented through a stepwise approach outlining the technology that has been developed and the technology that still needs to be developed to complete the overall system.

NOTATION

\[ a \quad \text{power index of breakage function} \]
\[ f_{ij} \quad \text{process feed mass flow rate} \]
\[ i, i' \quad \text{index variables for size classes, } i<i' \]
\[ j_1, j_2, \ldots, j_n \quad \text{index variable for physical property classes } 1, 2, \ldots, n \]
\[ k \quad \text{index variable for process output stream} \]
\[ P_{i_x} \quad \text{process product mass flow rate} \]
\[ B_{i_x} \quad \text{breakage function} \]
\[ I \quad \text{identity matrix} \]
\[ K_t \quad \text{constant in breakage function} \]
\[ OV_{i_x}, OV_{i'} \quad \text{device operating variables} \]
\[ P \quad \text{set of model parameters} \]
\[ S_{i_x}, S \quad \text{selection functions} \]
\[ T_{i_x} \quad \text{transfer coefficient} \]
\[ X_{i}, X_{i'} \quad \text{size class intervals} \]

to provide assurances that performance targets will be met and to optimise performance. Such testwork has often been neglected due to the high cost involved and has led to cases where full scale plant failed to meet expectations or specification. Further, the full environmental impact of the developed process has often proved difficult to predict.

A robust simulation model for waste treatment can aid the planning, design and operation of waste processing operations by providing a substantial part of the underpinning and necessary information, significantly reducing testwork requirements. The model can allow the conceptual design of plant, highlight uncertainties and sensitivities in the process flowline or flowsheet, provide comparison of process options and help trace pollutant pathways. It can also enable plant sizing, quantification of the effects of operational factors such as source separation, feed variability and equipment set-up and can further allow optimisation of the process against any objective criterion (such as maximising energy recovery). More generally, the modelling approach will help to reduce development risk.

Simulation models are now well proven in the chemical, paper and minerals industries but have, as yet, had little impact in the waste processing, although...
some pioneering work has been carried out, mainly in the United States.

An important precursor to process simulation is the establishment of the composition of the process feed, or proposed feeds to the process, at the required level of detail. This can become expensive in terms of the analyses needed. It may also be impossible to achieve logistically or with adequate representivity or in time. A means of estimating the necessary data independently, perhaps by utilising other data sources, then becomes essential. This estimation facility is currently being developed under the National Domestic Waste Analysis Programme. The complementarity of the national waste statistics and the process simulation method will provide an integrated tool which has many applications in waste and energy management. This integrated concept is shown schematically in figure 1. The concept is developed in this paper by stepping progressively through the technology involved.

2 WASTE CHARACTERISATION

A basis for domestic (dustbin) waste characterisation is provided by analysis of the waste by material component and size distribution. In the UK, six size fractions are generally used for this categorisation: +160 mm., -160+80 mm., -80+40 mm., -40+20 mm., -20+10 mm. and -10 mm. Eleven main material categories (table 1) are used but when a more detailed analysis is required, these fractions are further divided into thirty three sub-categories.

Table 1 Material categories of domestic refuse

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<td>11</td>
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The categories have been selected based on the experience and practicalities of sorting to provide generation rates for all the major recyclable components within the waste. The analysis itself is undertaken by hand-sorting a sample of the waste and screening each component by size. Practical considerations and problems of sample representivity constrain the size of sample that must be analysed. In normal circumstances, a full refuse disposal vehicle load of approximately 5 tonnes is treated. A 5% relative error on the analyses of most of the major components can usually be achieved, with this size of sample.

Chemical analysis of the whole sample, or of the sub-fractions, provides further information and detail on the composition of the waste. Determinations of the moisture content, calorific value, the contained volatile matter and fixed carbon ash levels provide the essential information on the 'energy value of the waste'. Analyses for heavy metals and for other key elemental components provide information on the potential toxicity of the waste. Further analyses for other toxins such as PCBs and dioxins are added if required.

Characterisation of waste to this level of detail is the minimum requirement for process simulation. It also defines the requirement for collecting the UK national statistics on the waste composition arising from households.

3 THE NATIONAL WASTE ANALYSIS DATABASE

The National Domestic Waste Analysis Programme (1) was set up by the UK Department of the Environment as a means of improving the UK's waste arising statistics, validating these data and developing a method of monitoring trends in waste arisings on a continuous basis. In the programme, a rationale was developed which will allow the correlation of domestic waste generation rates and waste composition (as defined above) with source details. These source details are currently based primarily on socio-economic information. The basis of this rationale will be expanded below. The Programme seeks to build up the base UK waste generation statistics through full characterisation of some 20 key selected waste streams each year over the Programme's duration. The data will provide a centralised, national reference facility, developed and held as a computer database at Warren Spring Laboratory.
3.1 Source characterisation

The National Waste Analysis Database uses the ACORN classification system to provide the primary basis for source categorisation. Developed by CACI, ACORN (A Classification of Residential Neighbourhoods) is a geodemographic classification system which allows census data to be classified into varying socio-economic types, according to the sort of residential area people live in.

An underlying assumption, of the Programme, is that people who live in similar neighbourhoods have similar purchasing and lifestyle habits and consequently will generate similar wastes. For example, low income households are low waste generators mainly because they purchase less and so there is little packaging etc. to dispose of. High income households are better placed to purchase luxury goods such as pre-packaged food stuffs, wine and magazines, which generate large quantities of waste high in paper and glass content. Although household socio-economic profile is not the only determining factor in waste generation, it has provided a credible and defendable starting point for the study. Other contributory factors affecting waste composition will be more fully detailed as the study progresses. These factors will include seasonal and regional differences, collection methods and the use of coal fires etc.

The waste arising and composition data, collected in the study, has been organised within the National Waste Analysis Database according to ACORN category (table 2), with each data set relating solely to a single ACORN source group. Each data set is further tagged with its date of collection, collection locality and collection method to allow for future developments.

3.2 Statistical models of waste composition

On the above rationale, the waste composition and arisings for any area (eg. enumeration district, city or region) can be estimated, to a first approximation, purely from the ACORN profile of that area. The waste composition will be compounded from the basic pure ACORN building blocks, stored in the database. For example, given an ACORN profile of 30% B, 20% D, 40% F and 10% J, the waste composition for that area is estimated by combining data from pure ACORN groups B, D, F, J in the same percentage proportions.

As more data is accumulated on measured waste compositions from a wider range of UK sources, the relative influences of all the contributory factors affecting waste generation will become better quantified. This will enable the creation of new statistical models and corrections to account, for example, for seasonal variations in weight arisings (eg. at holiday resorts), seasonal variations in waste compositions (eg. garden refuse content), regional differences (if any) between towns having similar ACORN profiles, and changes in consumer habit if the collection method is changed.

Although at an early stage of the overall programme, the base statistics and their manipulation through the simple models described above have already started to give assistance to Local Authorities: to more closely define waste arisings, to develop waste disposal and recycling plans and to improve contractual arrangements for waste management services. The evaluations of these options are still carried out off-line. The next, and important, step is to use the power of computer models and process simulation techniques to assist in the evaluation of, and in the optimisation of waste management strategies to meet set objectives.

4 PROCESS SIMULATION: MASS BALANCE PROCESS MODELS

Once the feedstock to any waste management process has been characterised (by direct measurement or through estimations according to the schema presented above) simulation techniques can then be applied to predict how this feedstock will actually respond to the process. Process, in this context, is defined in its

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Table 2 The ACORN classification system

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<tr>
<th>ACORN</th>
<th>Housing Type</th>
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<tr>
<td>A</td>
<td>Agricultural villages and farms</td>
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<tr>
<td>B</td>
<td>Modern family housing, young families</td>
</tr>
<tr>
<td>C</td>
<td>Older housing, intermediate status</td>
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<tr>
<td>D</td>
<td>Older terraced housing</td>
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<tr>
<td>E</td>
<td>Quality council estates, higher incomes</td>
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<tr>
<td>F</td>
<td>Council estates, older people</td>
</tr>
<tr>
<td>G</td>
<td>Council estates, inner cities, low income</td>
</tr>
<tr>
<td>H</td>
<td>Mixed inner metropolitan areas</td>
</tr>
<tr>
<td>I</td>
<td>High status non-family housing</td>
</tr>
<tr>
<td>J</td>
<td>Affluent suburban housing</td>
</tr>
<tr>
<td>K</td>
<td>Better-off retirement areas</td>
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</table>
broadest sense and may be anything from a simple selective collection (source segregation scheme) to a fully mechanised central waste sorting plant. The methodology for the simulation remains the same throughout.

The technical operation of each unit process, within the overall treatment, can be described mathematically in terms of a (mass balance) process model. Two main classes of model can be defined: (i) a separation model, where waste is separated into two or more discrete streams according to physical characteristics (eg. by particle size, density or magnetic susceptibility) and (ii) a transformation model where the waste undergoes physical or chemical change (eg. size reduction, pelletising, incineration etc).

Mass balance models for common mechanised sorting devices have been reported in the literature for more than a decade. These published models, which often have their origins in mineral processing technology, range from being purely theoretical to being purely empirical in nature. There is, however, little published data on just how well these models actually fit experimental observations. Some evaluation of the quality of the models has recently been undertaken by Warren Spring Laboratory, using both pilot scale data and data collected from commercial operations for reference. Although the results from the study can not be published for commercial reasons, the main conclusion can be disclosed: 'most models, as they stand, do not provide an adequate description of the process but they can be made to do so simply through empirical tuning.' This finding closely parallels the experiences of the mineral processing industry, where, arguably, the application of the simulation method has reached a more advanced stage and has several documented commercial applications (eg. 2,3). The 'phenomenological' modelling method that has been successfully applied to mineral processing plant, is outlined below. Reference is made to waste treatment applications.

4.1 Separation models

In sorting operations (eg. trommelling, magnetic separation, air classification etc.), the particle size and/or other physical characteristics of the particle will be important in determining that particle's response to sorting. The additional physical characteristics will, to a first approximation be implicit properties of the material type itself and can be regarded as constant within any material type. Paper and card, for example, have relatively low specific gravities whereas ferrous metal has a high specific gravity, the settling rates of plastic film are slow due to particle shape effects, ferrous metals have high magnetic susceptibilities etc. The relative importance of each of these physical characteristics to the separation is a function of the separating device used. For each separating device, separation performance can be described in terms of the fractionation of each size/ material class, from the process feed \( f \) to each device output \( p \). Mathematically this can be expressed as:

\[
P_{ij} = f_{ij} \cdot T_{ij}
\]

where the transfer coefficient, \( T \), is a function of the material category, the particle size and of how the separating device is operated. For each device, the following set of relationships can be formulated to describe the function \( T \):

\[
T_{ij} = f(T)\left(i,j,OV,P\right)
\]

\[
P = f_n(OV^*,P)
\]

The main model relationship (equation 2) comprises one or more equations formulated in terms of continuous functions of each size, \( i \), and of each physical property \( j \). Each material class is assigned a discrete value for each property variable, \( j \). The main model relationship also takes into account any operating dependencies \((OV)\) which can be quantified analytically. The effect of many operating variables, however, are very difficult to delineate and can depend, for example, on the exact fine-scale make-up of the waste. It would prove impossible to quantify these dependencies to high precision, although the underlying trends can usually be identified with reasonable clarity. These trend equations can be expressed as an auxiliary model relationship (equation 3). The link between the main and auxiliary model equations is a set of adjustable model parameters, \( P \).

The parameter set \( P \) provides the essential means for empirically tuning the model to match observation. Establishing the parameter set \( P \) provides the device model calibration. Calibration can be effected mathematically by regressing the model equations onto measured data sets, where available, to provide the closest (least squares) fit. Reference parameter sets can then be stored in a reference library to be drawn on when measured data is not available.
Once the calibration is established, equations 2 and 3 can be applied in a predictive sense, to estimate separation performance under different operating regimes. This is important, when it comes to optimising the process in order to meet specific processing objectives. This aspect will be developed further in section 6.

4.2 Size reduction models

Size reduction models (eg. for knife mills, hammer mills etc.), are based, in the first instance, on the breakage of homogeneous material. The models treat the size reduction process either as a single event or as a series of breakage events. In each breakage event, a fraction of the material is regarded as being selected for breakage and then broken into a distribution of smaller particles; the rest of the material remaining unbroken. The mathematical formulation of this process is usually expressed in a matrix form:

\[ p = B.S + (I-S).f \] (4)

Many functions have been proposed to fix the individual values in the selection for breakage matrix \( S \) and in the breakage matrix \( B \). An example of the type of function which is now being successfully applied to refuse size reduction is illustrated below. The quoted example refers to a function originally proposed some forty five years ago by Epstein (4).

\[ B_{0} = \frac{K_{0}}{S_{1} \left( \frac{X_{2}}{X_{1}X_{r+1}} \right)^{a/2}} \] (5)

The adjustable parameters in the equation are \( S_{1} \) (the value of the selection function for the top size class) and the index, \( a \). These parameters will take different values for each material category and, like the separation model parameters, must be empirically determined.

Comminution of composite materials often leads to total or partial liberation of individual material components. Liberation modelling, which has received much attention in mineral processing, has proved very difficult to model accurately. A simple approach, which appears to work reasonably, was developed at Warren Spring Laboratory (5) for gravity concentration circuits. It seems reasonable that similar models could be developed for operations in waste processing, although these models would probably need to be material specific (eg. targeted to a battery breaking plant, or to scrap wire recovery and so on).

4.3 Waste collection models

Mass balance models of waste collection schemes will provide a link, where necessary, between the waste arisings data and the waste processing models. The waste collection models will take exactly the same format as the mechanised sorting models and, as such can be fully integrated with them in the process simulator. The model functions are still adequately described by equations 1 to 3 above, with \( T \) now representing the diversion rate of a particular waste component to the collection scheme. Contamination of the collectibles by other material (eg. tin-plate in an aluminium can bank) is represented by non-zero \( T \) values for the contaminants. The operating variables, rather than being machine settings, will relate more to the geodemographic factors associated with the catchment area.

Prototype (probability) models can be built from analysis of the monitored performance data of the various collection schemes already in operation.

It must be borne in mind, when applying collection models, that the input (waste generation) data might itself be a function of the collection scheme. Corrections for this must be applied to the raw data rather than to the model. The modelling of these corrections has already been discussed in section 2 above.

5 PROCESS SIMULATION: OTHER MODELS

Chemical analysis data can be overlaid onto the mass balance models to enable predictions of the chemical composition, or energy value, of each separated waste component. Much of the chemical information that is needed will be available from the National Waste Analysis Database, though not always at the level of detail required for the simulation (ie. as separate analyses for each individual size/ material category). Full analyses, where available, will however provide base data relating to the typical chemical partitions within the waste. It may then be possible to apply these data more generally and to upgrade partial analyses through the establishment of suitable scaling factors.

In the simulation of sorting processes, a good first approximation towards solving the chemical balance is the assumption that the chemical composition of each size/ material fraction of the sorted product is the same as that of the equivalent fraction in the process feed. This implies that each sub-fraction is fairly
homogeneous in content and that separation is not biased significantly by material variations within that fraction. The accuracy of the chemical simulation will thus improve when a finer division of material categories is used (i.e. the categories become more homogeneous). In this respect a 33 category representation should furnish more accurate composition predictions than would be achieved by using a coarser resolution of 11 categories. This method of prediction would, however, be totally inappropriate for some specialised sorting processes (e.g. cadmium partitioning in the selective collection of Ni-Cad batteries), and an alternative approach would need to be found in these instances.

There are also many difficulties in predicting chemical partitioning in size reduction processes. As with the mass balance models, the inherent problems are linked to the possible heterogeneity of the comminuted fragments. This is clearly an area for further focused fundamental research.

Energy models can also be built for each of the unit processes. In the simulator these energies are cumulated to provide the total power consumption data. Energy models and raw consumption data are available from the published literature and from equipment manufacturers. It must be borne in mind here, that in assessing total energy consumption, material transport requirements should also be included within the overall process. This may necessitate the construction of additional sub-models, e.g. for conveyor belts.

Economic models may also be applied. These models essentially cumulate capital, installation, finance, labour and maintenance costs of process operations or refer to the revenue and disposal costs of the processed products.

6 PROCESS SIMULATION

Process simulation is the computer representation of what happens, or might happen, in a real process. In the current context, process simulation provides a description of waste treatment operations involving one or more coupled unit treatment processes (or process flowsheet). The flowsheet comprises a network, or line, of nodes with connecting flow streams. Each node denotes a unit process, represented within the simulator by a mass-balance process model. The mathematical solution of the flowsheet adopts techniques originally developed in the chemical engineering industry. A review of these techniques is given by Westerberg et al. (6). Solution of the flowsheet involves partitioning the circuit into its constituent loops and iteratively solving each loop and each of the models contained therein. As the waste management models are generally non-linear in format, and cannot easily be linearised, a serial solution method is preferred.

The Warren Spring Laboratory simulator GSIM (5), developed originally for mineral processing applications, contains two important additional features: (i) flow constraints can be set and (ii) the circuit operation can be tuned to optimise overall process performance against a given objective criterion.

A large number of variables can affect circuit performance. To establish the optimum combination of these variables requires the application of a numerical search algorithm. In GSIM, a pattern search method has been chosen (4), although a derivative-based method could equally suffice. The objective criterion against which the process performance is judged will vary according to application. In waste processing, this objective function might be to maximise energy recovery, to maximise recovery of a recyclable component or of the total recyclables and so on. Constraints might also be set, for example a cost ceiling, or an emission limit or a 25% recycling target. Care must be exercised when setting these objectives depending on the quality of the models themselves. Optimising on technical objectives should generally produce more robust results than would optimising against economic objectives.

7 STATE OF THE ART

The concept presented in this paper is ambitious. A prototype (validated) integrated system is, however, not that far from realisation. Much of the modelling and database technology has already been developed, some of it as much as forty five years ago. Also, enough data now exists, both with regard to waste characterisation and with regard to process or collection performances, to make application industrially viable. The innovation lies in assembling the technologies into an integrated whole and validating the methods against documented measurement.

There are still, of course, many gaps in the data and in our overall understanding. As knowledge grows, these gaps can be progressively filled. For example, civic amenity waste and commercial and
Industrial wastes are not categorised to the same extent as domestic wastes. A General Industrial Waste Analysis Programme, sponsored by DTI, is, however, now under way and should furnish some of this information. Further fundamental work needs to be carried out on model development, to introduce a wider range of models and to refine the current models. Particular attention needs to be given to broadening the validity of chemical partition models.

REFERENCES

(4) EPSTEIN, B, The mathematical description of certain breakage mechanisms leading to the logarithmic-normal distribution. Journal of the Franklin Institute, 1947, 224.

ACKNOWLEDGEMENT

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Fig 1 Schematic representation of waste management model