Programme Area: Bioenergy

Project: Energy From Waste

Title: Systems Model Development Report

Abstract:

This deliverable is number 2 of 3 in Work Package 3 and describes the work carried out to October 2010 in the development of the component technology and systems models. The report summarises the development work done to integrate into a single system level model the individual component technology models for each of the main pre-processing, processing, post-processing and power generation components which may be expected to comprise an end to end energy from waste system. The development work is based on both literature and test results from the Energy from Waste project, detailed in deliverable 2.2.

Context:

The Energy from Waste project was instrumental in identifying the potential near-term value of demonstrating integrated advanced thermal (gasification) systems for energy from waste at the community scale. Coupled with our analysis of the wider energy system, which identified gasification of wastes and biomass as a scenario-resilient technology, the ETI decided to commission the Waste Gasification Demonstration project. Phase 1 of the Waste Gasification project commissioned three companies to produce FEED Studies and business plans for a waste gasification with gas clean up to power plant. The ETI is taking forward one of these designs to the demonstration stage - investing in a 1.5MWe plant near Wednesbury. More information on the project is available on the ETI website. The ETI is publishing the outputs from the Energy from Waste projects as background to the Waste Gasification project. However, these reports were written in 2011 and shouldn't be interpreted as the latest view of the energy from waste sector. Readers are encouraged to review the more recent insight papers published by the ETI, available here: http://www.eti.co.uk/insights

ETI Energy from Waste FRP Project

Deliverable 3.2
System Model Development Report

Final as Submitted to the ETI
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Executive Summary

The report, Deliverable 3.2 of the ETI's Energy from Waste FRP project this is an activity report, describing the work carried out to date in the ongoing development of the component technology and system models.

The report describes the development of the component technology models, both those based on literature only and those based on the experimental work carried out for this project. It has been recognised that there are missing linkages between the present models and the data developed from the experimentation.

The development of the component technology models, especially those based on the Cranfield test data, has proven difficult due to the variation of the results and the single experiment undertaken per feedstock and technology. The products that are produced, though consistent in what they are, differ to the extent that they are evolved. In addition, particularly in the gas phase, there are some products that may have been produced but which have not been analysed, such as C2 and C3 molecules. It will be necessary to have further communication and discussion with the experimental team to identify a way of adding further robustness to the models developed in the thermo chemical assessments. A meeting is being scheduled between the modellers and experimenters for mid-August to assess the data, and propose any further experiments which would add confidence and value to the model.

The report also describes the development of the system level architecture, which uses a common set of variables to transfer data between the different component technology models. The system model also incorporates a user interface, which may be used to select technologies which may be considered by the model to comprise the system configuration. The system model has been shown to be functional, in that it simulates the components in order, based on the selected material feedstock and feed rate. To date, the system model has been tested to ensure operation only. As an outcome of the component models, the system level results require further assessment. Further discussion and liaison between all relevant parties will be required to produce the final working offering. All the models finally developed must be used with a level of caution that the inputs and outputs must be carefully assessed and validated against what would have been expected.

A separate seminar has been undertaken by the consortium in mid-September to go through the model and explore the other variables and assumptions to further aid model robustness. The outcome of this seminar, alongside further model development will allow for the subsequent sensitivity analysis and variable optimisation planned for Deliverable 3.3 of this project.

Report Compliance

This report forms Deliverable 3.2 in the ETI's Energy from Waste FRP project. The agreed contents of this report, as defined in Schedule 1 of the project Technology Contract are:

One (1) electronic copy and one (1) printed and bound copy of a report will be submitted to ETI. The report is expected to be between 10 and 20 pages of text plus references and to contain:

- An executive summary
- A description of the methodology for system modelling, including
- Modification and presentation of data from work package 2
- Presentation of modelling results
- An explanation of the integration process and solver code generation
- Description of methodology of, and conclusions from, validation of model performance
- Summary of system models
- Presentation of modelling results
- Identification of the requirements for further technology testing (if any) to validate system model performance
- Conclusions
- A full list of references

This report will enable the ETI to satisfy itself that appropriate modelling methodology has been established to enable the robust analysis of Energy from Waste system performance, both for the current state of the technology (assessed in 3.2) and for optimised technology systems (to be assessed in 3.3). This report will also identify the requirements for further technology testing (if any) to validate system model performance. System models created in Matlab will be provided as .mdl files. System models will be combinations of "black box" component models, with hidden underlying equations (background IP). Input parameters to the models will be user configurable via an Excel input/output user interface.

The report, Deliverable 3.2 of the ETI's Energy from Waste FRP project this is an activity report, describing the work carried out to date in developing the component technology and system model. Due to the developmental nature of the model in its current form, this report does not include a discussion of the model results. To date, the system model has been tested to ensure operation only. The results generated are under scrutiny, and investigation is ongoing into the source of some spurious results. This investigation is revealing the need for further model development, which will be carried out in the initial stages for Deliverable 3.3. As such, the results have not been examined in detail or compared to other sources (e.g. literature). The consortium have scheduled a model seminar in mid-September to run a range of scenarios with the model to check and compare the results and model robustness, prior to carrying out the system sensitivity and optimisation analysis for the identification of high efficiency systems and development opportunities.

Introduction

The ETI Energy from Waste project seeks to examine the technology development and demonstration needs to allow a wide range of wastes to be used to generate electricity in the range of 1 to 10 MWe. To achieve this, the project is investigating UK waste arisings with a view to their energy content and processing needs (Work Package 1) and the operation of efficient processing technologies utilising these wastes (Work Package

2). These aspects will be combined into a system level model to simulate different system configurations operating on a range of mixed wastes (Work Package 3) to identify the lowest cost energy systems, both current and those which could be developed, for the use of wastes as a low carbon energy resource (Work Package 4). This report accompanies the initial system model to form deliverable 3.2, and outlines the development of the component models based on the test data obtained from Work Package 2 and the combination of these component models into a system level model.
The technology component models are based on the physical and/or chemical transformations which occur within each technology, as most appropriately models the technology's operation. Each component technology's output is dependant on the process which occurs within the technology, and its inputs, to generate the component outputs.

Technology Component Model Development

Component technology models for each of the main pre-processing, processing, post-processing and power generation components which may be expected to comprise an end to end energy from waste system were initially developed produced for Deliverable 3.1 of this project. These initial single component models were based on literature data and consortium know-how, and were not validated, nor combined into a system of multiple component technologies.

There is still a gap between the models developed at present and the final wok up of data from the experimentation. The modifications made at present are an approximation based on the raw data that has been delivered. A further round of discussions is to take place between the modelling team and the experimenters to attempt to bring them closer.

The subsequent step to the initial model development was to combine the component models into an end-to-end system model, where the outputs from one component model could be read as the inputs into the following component model. The development of the system model is described below. In parallel to the development of the system model, the individual component models were further developed in light of the test data generated in Work Package 2 of this project, and to refine their operation on a system level.

Waste Materials Properties Database

The system model calculates the energy generation potential from waste materials, given a certain throughput, which would be a function of material availability at a location. To do this, the first "component" on which the model draws is a database of materials and their physical and chemical properties. The values in the database are those that have been measured and analysed from Work Package 1 (Waste Assessment) of this project where possible. Any energy from waste system requires both the physical and chemical transformation of the feedstock material into a secondary fuel stream, and then into electrical (and heat) energy. To accurately reflect these transformations, the component models manipulate both the physical and chemical aspects of the materials as appropriate to reflect the real-world operation of each technology. The material properties database includes a range of material properties which reflect the physical aspects of their processing. These properties include the material toughness, which determines it's resistance to shredding, and a general

representative “particle size” for each material. Another property included is a “digestability” index, as the Anaerobic Digestion model currently does not discriminate between in-organic and organic materials, and as such would indicate a gaseous output from any material. This digestability index is used to define those materials which may be digested. Further development of the properties database and model would allow for the appropriate characteristics to be present in the database, and referenced by the model. In particular, the toughness of materials has not been measured experimentally, though has been found to be a considerable issue in their pre-processing for the gasification tests carried out for this work. The values currently in the database are based on estimated values based on this experimental experience, and the model would benefit from better empirical data on the energy requirement for material processing.

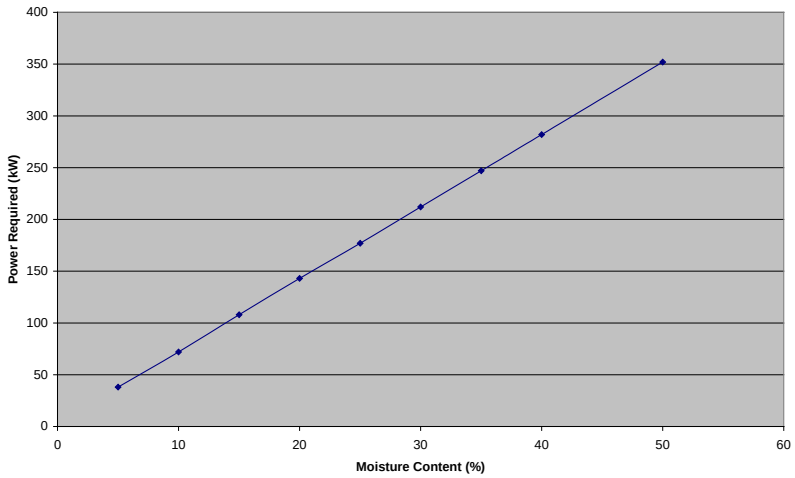
Seasonal Effects on System Models

The models as previously stated work upon the elemental analysis of the products to perform the mass balances. They only differentiate between materials on this basis. The models assume that these are thermo chemical, biochemical and thermodynamic processes.

From the waste analysis in the 1.2 report (admittedly only identified from Season 1 and 2 samples). It is apparent that there is very little variation in the ultimate elemental analysis of the waste materials that would be processed. Processed, means the materials that would be used in the technology for the production of fuel (such as AD unit, gasifier, pyroliser etc.), this includes sorting and drying requirements. When adjusted to take account of inert materials and moisture the Carbon content of materials averages 49.4% with a deviation of 5%, while the hydrogen averages 5.6% with a deviation of 1.5%. Some concern may be raised about the analysis of one or two of the samples which could make the results tighter. The strongest effect on the make up of the waste materials is the incorporation of the Inert/Agg/Soils that appears in some batches and the moisture content of the materials. It is feared that the waste arisings are so variable that no true correlation between the waste make up and the season is possible to produce.

The variability in arisings shown in the Cranfield report will have a significant effect on any particular installation. The ability to turn up and turn down the facility to meet the inputs will be a critical factor. The turn up and turn down of the process may be required to be a scale out approach of turning units on and off.
In the present models and from the work so far in the experimentation it is difficult to identify a major difference in the materials and the elemental analysis is the important factor for the operation of the reactors.

It is proposed to show the effect on moisture as a parasitic load on the facility. A system model can be run using a high moisture load and one with a low load.
The effect of variability of throughput it is proposed to shift this through to the 3.3 report being part of the sensitivity analysis.



Based on a 1000 kg/hr throughput the parasitic load that moisture content would have on a thermochemical process.

Pre-Processing Models

Shredder Model

The initial shredder model was further developed from the initial model to reflect the operational energy requirement and machine cost relationships to the material throughput. The model is based on the sales literature for the range of commercial waste shredders manufactured by Untha, used to shred the materials for the test work (Work Package 2) of this project.

The shredding of a material involves breaking the material through either “ripping” or “cutting” actions. These ripping and cutting forces are exerted on the material by blades or teeth on the periphery of a rotating drum. Three designs of shredder exist with different configurations of cutter drums, these are single, twin and four shaft.

In a single shaft machine, the cutter bar sits at the lowest point at the side of a wedge shaped vessel. A ram runs along the open base of the wedge and forces the material onto the cutter bar. A twin shaft design utilises a pair of interlocking cutter bars places along the gutter of a vee-shaped vessel, and uses gravity to force the material onto the cutters. Some of the teeth in such a design are hooked shaped to pull the material onto the cutter bars. Four shaft machines are similar to twin shaft designs but have a pair of toothed drums located above the cutter drums to pull the material through the device. In all cases, a screen with holes of a defined diameter is places below the cutter drums. This screen allows the passage of material which is below the hole size, whilst larger material is swept back to the cutters for further size reduction.

For a given machine size, the material throughput is dependant on the screen hole size, and the waste “shredability”. This material property is difficult to define as it incorporates elements of material hardness, brittleness and toughness. In turn, the energy consumption required to shred the waste is dependant on the material throughput as well as its shredability. The cost of commercially available shredders is dependant on the model range as produced by manufacturers, and hence is limited to discrete values. For the purposes of this project it was required to define a generic, material throughput

dependant cost which would indicate the capital cost of the equipment to process the material.

Machine specifications from the full range of single, twin and four shaft machines manufactured by Untha were copied into an Excel spreadsheet. This range of machines covers the full range of material throughputs of relevance to this project, from 2 to 180 m3/hr. The specifications include the maximum rated electrical energy consumption of the driving motor(s), the hole screen size range available and the nominal material throughput. Through personal communications with the UK distributor for these shredders, nominal machine costs were also added for each model. For range values, such as those of the screen hole sizes available, median values were used in subsequent calculations.

Whilst the nominal and maximal values given in the machine specifications provide an overview of machine capabilities, they do not account for the real-world operation of the machines, at lower duty factors. To compensate for this, an engineering judgement factor was added to the spreadsheet model to account for operation of the equipment with no material loading. The waste is assigned a shredability factor, which is used to calculate the loading on the machine, and in turn the actual material throughput. The throughput calculated for each machine is that based on the material loading up to the maximum specified throughput, above which the maximum throughput is used. Similarly, the machine energy consumption is reduced by the waste loading factor for lower material throughputs.

For each machine, the actual energy and costs are calculated for the actual throughput, given the waste “toughness” and raw particle size property from the material properties database and the desired output size. The equations for the curves which intersect the range of commercial machines are calculated, from which the theoretical energy consumption and cost can be calculated for any theoretical size machine. In the subsequent sensitivity analysis, system energy consumption can be assessed in relation to screen size, where the generated particle size has an effect on the subsequent processing technology.

Sprinkler Model

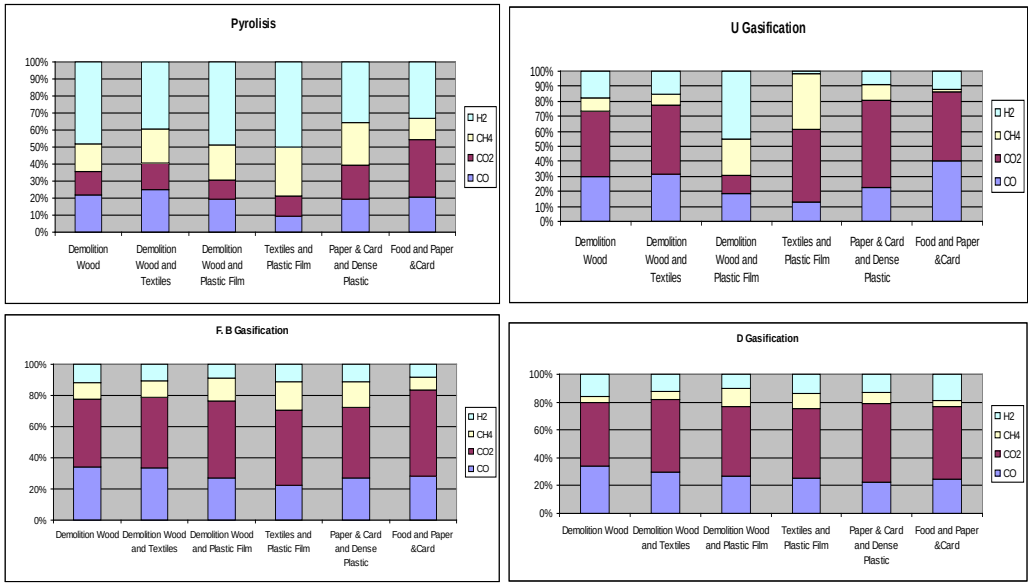
The processing of organic wastes by anaerobic digestion is likely to require the addition of water in practice to enable microbial movement. In reality, this water would be added either in a separate chamber to also enable feedstock pumping, or in the digestion vessel once the feedstock has been loaded by other means. To represent both of these situations, a sprinkler model has been developed. This model uses the difference in required moisture content in the anaerobic digestion process, which is a variable currently set at 50%, and the feedstock moisture content to calculate the amount of water required to be added. The energy demand of this component is determined from the pump energy, and the cost of water is a variable, currently set at 0.06p per litre, based on an assumed commercial value of water which retails at 1p for 10 litres [5].

Drier Model

The drier model has not been required to be developed. However, the assumption has been made that the energy required to evaporate off the moisture is supplied thermally (from excess process heat), and as such that there is no electrical demand from this component.

Work Package 2 Data

Cranfield have performed experimental work on the technologies of gasification and pyrolisis. Below is a modification of the data produced to show the products of the processes with the inerts, such as nitrogen removed.



The more 'intense' the processes that are performed on the feeds the relatively more consistent the results. The CO_2 levels are higher in the gasification proesses, most probably providing the energy to drive the processes. Though in the pyrolisis process there will be an increased oil production not shown here.

Processor Model Development Incorporating Cranfield Results

To generate data for a range of thermal technologies operating on waste materials, Cranfield University have performed experiments in Work Package 2 of this project. For the current deliverable, CPI have attempted to incorporate this data into the models previously developed (Deliverable 3.1) to give some further validation to the models for use in predicting the potential fuels arising from the waste feed stocks and the potential technologies used. However, due to the single set points and repetitions of the experiments, it has been found difficult to develop true correlations or behaviours of the feed stocks in the different process experiments undertaken at Cranfield. For example, the feed materials, by their very nature of being from mixed waste streams, are inconsistent and vary greatly. The products that are produced, though consistent in what they are, differ to the extent that they are evolved. In addition, particularly in the gas phase, there are some products that may have been produced but which have not been analysed, such as C2 and C3 molecules.

To try to give some alignment between the models and experimental data, the models have been adjusted using constants and factors to adjust the components of the gas streams. In addition, the tars output of the models has been simplified on the assumption that any compounds present in the gas stream are either oxygenated, and thus assumed to be phenol (C_6H_6O), or un-oxygenated and assumed to be $C_{10}H_{12}$.

All of the thermo chemical processes investigated at Cranfield show a significant amount of carbon dioxide in the product gases, with the more intense treatment processes increasing the quantity of carbon dioxide. The technologies investigated have used air for injection while some use inert gases or steam this may reduce the carbon dioxide and may be worth investigating experimentally should further tests be carried out. The use of steam as the fluidising/gasification medium, even for smaller scale technologies, may provide a unique development opportunity, although the cost-performance trade off for this would have to be further examined.

Model Layout

The component technology models were developed in Excel spreadsheet format. An input/output sheet was added to more easily identify the factors that influence the outputs of the process.

Feeds

The component models still require the elemental make up of the feed to be specified, which can be input from the material properties as assessed in Work Package 1 of this project. The materials assessed by Cranfield have similar make up to the biomass materials that have been used in the models previously, which allows a direct substitution into the models. However, caution needs to be taken if some values are low, such as hydrogen, as the product totals are taken to be fractions of the feeds and concentrations taken as average from the experiments. This can lead to negative numbers and a check is required.

Anaerobic Digestion

The model now contains the capability for the addition of $FeCl_2$ for the reduction of hydrogen Sulphide. The model calculates the amount of ferric chloride on the expected H_2S production. It should be remembered the alternative to this chemical addition is off gas scrubbing. The model originally used the feed rates to calculate the methane production. In the spreadsheet model, cell C34 was a check calculation based on references of actual installations. Potassium and phosphorous addition is calculated by adding potassium phosphate to achieve a specified NPK ratio. The model reacts the evolved ammonia with sulphuric acid to remove it as ammonium sulphate. Another potential source of the ammonia is the relatively high nitrogen content of the feed material. Adjustment of this would give a lower ammonia production. Consideration of this should be made when actual feed material to be used is identified. There is now a small calculation that defines the amount of the produced methane would be needed to maintain the operating temperature. This is arrived at by dividing the ambient losses and dividing by the heat of combustion of methane.

Fluidised Bed Pyrolysis

In the fluidised bed pyrolysis model, the feed is assumed to breakdown in the pyrolysis process to bio oil, gas and a char residue. The percentage splits of the oil and gas as a weight percentage of the dry feed is then inputted. The composition of the bio oils are

taken to be either phenol or $C_{10}H_{12}$ to identify oxygenated or un-oxygenated materials respectively. The proportion of the outputs can easily be modified in the spreadsheet structure if subsequent data should indicate different output component proportions. The composition of the bio oil can also be developed should further laboratory research data become available. The oil composition is broken down elementally in the spreadsheet to allow for further calculation in the spreadsheet for the mass balance. The gas fraction is specified in the input page based on the data from the experiments. At present there are no C2 or C3 molecules specified, although they are retained in the spreadsheet structure to allow for future incorporation. The gas composition is broken down elementally in the spreadsheet to allow for further calculation of the mass balance. The composition of the Char is determined from an elemental balance on the system. As such, if either the feed elemental composition or the bio oil produced changes, the char composition will adjust. An estimation of the heat required to drive the process (pyrolysis is essentially an endothermic process) is also made. The heats of formation of the products are subtracted from those of the feed materials. This is the heat then needed to be used in the process, in this case from the re-circulating sand. The amount of sand re-circulating is estimated from the heat needed for the process and an assumed temperature drop of the sand when in the reactor. The energy of combustion of the char is calculated from a correlation developed by NREL [1]:

$$HHV = 146.58C + 568.78H - 51.53(O+N) - 6.58A + 29.45S$$

This correlation gives the heat of combustion in units of BTU/lb from the Wt% of the elements in the char. The temperature is then calculated using an estimated specific heat capacity. This shows that the whole process can have an energy surplus when the Char is combusted. Although the model appears to operate satisfactorily, further refinement of the model would be desirable based on a more comprehensive data set (e.g. range of temperatures for each material).

Rotary Kiln Pyrolysis

This component model spreadsheet is essentially the same as the fluidised bed pyrolysis spreadsheet, although in it the lack of re-circulating sand means that only the heat required to be delivered to the rotary kiln is calculated.

Updraft Fixed Bed Gasification

The approach to modelling the fixed bed gasifier is similar as for the pyrolysis models. In reflection of the main reactions occurring in a gasifier reactor, the model partitions the unit into four sections, drying, pyrolysis, reduction, and oxidation. A mass balance is then performed across each section. Each section is seen as a black box and no account of reaction time or dynamics has been incorporated. The feed to the gasifier is inputted as an elemental balance. In the first stage, drying, residual free moisture is driven from the feedstock entering the gasifier based on a simple split with an energy demand coming from the exit gas. The second stage is a pyrolysis stage where oils and some of the produced gas are driven from the feed material. The gas produced does not contain C2 or C3 molecules as per the Cranfield data though the calculation connections are still in the spreadsheet. The oil is again simplified to either phenol or $C_{10}H_{12}$ for oxygenated or un-oxygenated products. The weight percent of both the oil and gas as a percentage of the dry feed stock are inputted based on the test data. Again, care must be taken not to

drive some of the values to negative numbers. An elemental balance is performed to calculate the solid material continuing down the gasifier. If the carbon and hydrogen content start to go too high or too low the model may produce results that are inconsistent, although it should be possible to interchange both the feed stock elemental content and the pyrolysis products and still attain a credible result. The third stage is modelled as a reduction stage where water produced from char combustion (or additional injected water from steam gasification) reacts with the carbon in the solid char phase to produce the gas. The model has been developed to now react a fraction of the water available to gas. This fraction is adjustable as the reaction is endothermic, thus if too much water is reacted, unrealistically low temperatures are created in the reaction mass. The final zone is the oxidation zone where the residual char is burned to provide the process heat, again using the NREL correlation stated above. The stoichiometric excess of the air is specified, this can be less than that for complete combustion of the char. Again this combustion has an effect on the calculated temperature profile in the reaction mass. It should be noted that the enthalpy calculations used in this model are relatively crude and are presented to give an indication of temperature profiles only. Due to the unknown enthalpy values of materials and the assumptions in the calculations, the energy balance proved to be the most difficult part to model and for a more accurate temperature profile each zone would be required to be broken down into more elements, although this would unnecessarily complicate the model for the outcome of this project. In the reduction zone, the temperature drop of the endothermic reaction is calculated from the difference in the heats of formation of the water reacted and the carbon monoxide produced, based on estimated heat capacities of the materials. A similar approach is performed in the pyrolysis and drying zones which both are net users of energy. Finally an assessment of the solids temperature is made by assuming that it matches the gas temperatures; a value of the average temperature is calculated for completeness.

Downdraft Fixed Bed Gasification

The approach to modelling the fixed bed downdraft gasifier model is similar to that taken for the updraft gasifier, in that it also partitions the unit into four sections; drying, pyrolysis, reduction, and oxidation. A mass balance is again performed across each section and each section is seen as a black box no account of reaction time or dynamics has been incorporated. Although the model is split into four sections, the solid gas and liquid phases are in co-current motion through the reactor. In effect in the downdraft process the reaction zones would be smaller and more intense than the updraft process. The feed to the gasifier is input as an elemental balance, which works as the waste materials generally have a similar elemental make up as the biomass on which the model was originally developed for Deliverable 3.1. In the first stage (drying), residual free moisture is driven from the feedstock entering the gasifier, based on a simple split with the energy demand being satisfied by the exit gas. It is assumed the water becomes free and is thus able to react separately. The pyrolysis stage is modelled in a similar way as for the updraft gasifier, and similar comments apply. Due to the nature of the reactor, it is assumed that the oils and gases produced are free of solid mass and hence able to travel and react independently. In the reduction stage it is assumed that two reactions are possible; the production of gas from water and carbon in the char, or the reduction of carbon dioxide in the gas by carbon in the char to produce carbon monoxide. The input sheet allows the specification of the ratio of these two reactions. The input sheet also allows specification of how much carbon in the char is consumed in these reactions, which is likely to be a function of the temperature achieved in the reactor bed, although

the level of calculation to asses this is beyond the scope of this modelling. The final zone is the oxidation zone where the residual char is burned to provide the process heat. An air excess is assumed in the feed. At present all tars are assumed to be converted to carbon monoxide, carbon dioxide or hydrogen. The fraction of char remaining can be specified. As for the updraft gasification model, the enthalpy calculations used in this model are relatively crude and are presented to give an indication of temperature profiles only. As for the updraft gasification model, the energy balance in the reduction zone is calculated, as are the temperatures of the outputs.

Fluidised Bed Gasifier

The fluidised bed gasifier is a direct contact technology where the material to be gasified is in direct contact with a hot heat transfer medium, such as sand. The spreadsheet has been developed from that produced for Deliverable 3.1, which was based on work performed by the NREL [2]. The gases that are produced are a function of the temperature that the process is being performed at, with the relationships being second order polynomials. In addition, the amount of char that is produced is a function of the reaction temperature. If the char is combusted, it can be seen that equilibrium will be reached. That is, at lower temperatures more char is produced which will release more heat when burned, increasing the process temperature, and at higher temperatures less char is produced, thereby generating less heat when burned. As for the other gasification models, the feed to the gasifier is inputted as an elemental balance, and as stated above as the waste materials have a similar elemental make up as the biomass on which the model was originally developed. The other inputs are the expected operating temperature, an estimate of the volume of sand re-circulating and the fluidising gas as a fraction of the feedstock. In the first iteration, these are maintained as constants based on values for which the Cranfield test data is consistent. The spreadsheet calculates the gases and tars generated and the char produced. As the spreadsheet cannot work in a loop, a solver is used to calculate the return sand temperature after char combustion, and the excess energy available at this temperature. The values of gases produced are consistent when the temperature that the fluidised bed gasification experiments were performed at Cranfield is input. Whilst the original model was based on steam gasification of biomass, the use of air as the fluidising medium, as at Cranfield, increases the consistency of the results further as carbon monoxide will be oxidised to carbon dioxide. The results of the fluidised bed gasification are also relatively consistent across the different feed stocks, leading to the conclusion that the present spreadsheet is applicable to this process.

Conclusions

The original component models of the thermochemical technologies developed for Deliverable 3.1 of this project were based on biomass systems. The experimental data from the tests performed at Cranfield University show good correlation to the original correlations, and hence the models have been able to be suitably adjusted to give similar results to those from the experiments at Cranfield. However, due to the limited number of data points to which the models are fitted, there are more constants and assumed fractions than there would be in better understood systems. The spreadsheets can be used to give an indicative assessment of what potentially can be produced from the waste fuels in terms of the main outputs that would be of interest for use of the gases for power generation; namely oils, tars, carbon monoxide, carbon dioxide, hydrogen and methane.

Post-Processor Models

It was recognised that the post-processing technologies for which models were initially developed were those to process gasification derived gases. However, no models were developed to post-process the gases generated from digestion, in particular to remove the H_2S from these gases. To address this, some simple models were developed for chemical absorption, pressure swing adsorption, cryogenic separation and membrane separation based on reference [4]. In addition, the water scrubber model was developed to remove a proportion of H_2S from a gas. For each of these models, the energy requirement was deemed to be based on that to drive motors for pumps and fans, with an average value of 0.06 kW/kg of material pumped being used to derive the energy demand for each model. This value is based on engineering judgement, and would need to be further validated based on test data.

Energy Generator Models

Gas Engine

For the previous deliverable of this Work Package, a number of discrete models were developed to represent a range of current Caterpillar engines which may be considered for such applications. However, the intension for the project deliverable is to indicate overall system performance at any scale relevant to the waste material throughput. As such, it was desired to develop a single model to generically represent engines at any scale. To enable this, a new generic gas engine model was developed based on the single cylinder engine tests which were carried out in Work Package 2 of this project. This model uses the thermal efficiency and high level combustion characteristics to determine the engine outputs (heat and power) and emissions. As such, the model developed for this project is considerably more basic than a full engine model. However, the development of a full, validated engine model is a considerable task and beyond the scope of this project. However, as described below, it is intended to enable the potential integration of the full engine model into the Energy from Waste system should such a model become availableto more accurately represent engine operation, and emissions outputs, when using these gases.

Fuel Cell (Molten Carbonate)

The fuel cell model developed for Deliverable 3.1 has undergone major development to better reflect the operation of the technology. A full model development report for this model is included as an appendix to the report.

Technology Costs

To allow scalability of parameters, all component technology costs are normalised on a kg/hr capacity basis, where the kg refers to the mass of the input stream (e.g. material input, gas input), with the exception of the power generators which are normalised on their electrical energy generation capacity (e.g. per kWe capacity). To derive the actual capital costs and operational costs, the normalised costs are multiplied by the throughput for each component. In recognition that smaller scale equipment is typically more expensive on a capacity basis, the relationships of the costs to the throughputs are not necessarily linear, and are based on the equations of curves which best fit the available cost data gathered for this project. However, the technical and commercial

scarcity of many of the technologies of interest means that much of this cost data is based on relatively few data points, and further assessment is required of the system model outputs to check whether total system costs generated are sensible to scales of waste processing capacities input into the model.

System Model Development

The system model incorporates the component technology models into a single end-to-end system process model. To aid compatibility between the component models, all component models were converted into the Matlab modelling code structure, based on their development as Excel spreadsheets as detailed above. Conversion of the spreadsheet models into Matlab comprised of translation of the model variables, and the formulae which manipulate the physical and chemical parameters to represent each technology's operation. Additional parameters of capital and operational costs were also added to the Matlab versions of the component technology models.

To enable transfer of variables between models, a set number of defined variables were defined which covered all of the inputs and outputs which may be relevant to all the models. These variables include a wide range of gas constituents to cover all those generated from the models, and the associated properties of the gases, as listed below.

CH_4(kg/hr)	N_2(kg/hr)	tars(kg/hr)
CO_2(kg/hr)	O_2(kg/hr)	particulates(kg/hr)
CO(kg/hr)	H_2S(kg/hr)	solids(kg/hr)
C_2H_4(kg/hr)	SO_2(kg/hr)	wobbeindex
C_3H_6(kg/hr)	NH_3(kg/hr)	LHV(btu/lbm)
H_2(kg/hr)	HCl(kg/hr)	fuelflowrate(MW)
H_2O(kg/hr)	C_2H_2(kg/hr)	temperature(C)
NO_2(kg/hr)	oils(kg/hr)	

These variables are held in a matrix, with each value being updated as the stream passes through subsequent technologies and hence mathematically manipulated. The model cycles though every possible combination of selected technologies. The intermediate and final results are published to a CSV (comma separated variable) file, where they can be manually analysed and ordered to select the best system based on the user's requirements. The main values that are calculated are the thermal and electrical energy demands of the system, the thermal and electrical generation of the system and the net difference between these, as well as the system capital and operational costs (including feedstock costs).

The overarching system model uses a combination of user defined parameters and pre- and post- processing technology requirements to calculate the process technologies, and their operational performance. In developing the system model, attention was paid to the future development, expandability and usage of the model. To enable this development and usage, some features are included in the model which are not usable in the version that accompanies this report but which are visible for ease of incorporation into future developments of the mode. Each step in the system model operation methodology is described below, which also illustrates the system model architecture.

System Model Operation

The user is required to save all 27 ".p" files and 2 ".fig" files into the same directory (folder). The ".fig" files should not be opened directly. From the Matlab main window, the directory that contains the model files should be opened. When all the files are visible from within Matlab, the user is required to type the command "`EfW_Main`" into the Matlab command window. This brings up the main Graphic User Interface (GUI) which is used to control the system model, as shown in **Figure 1**.

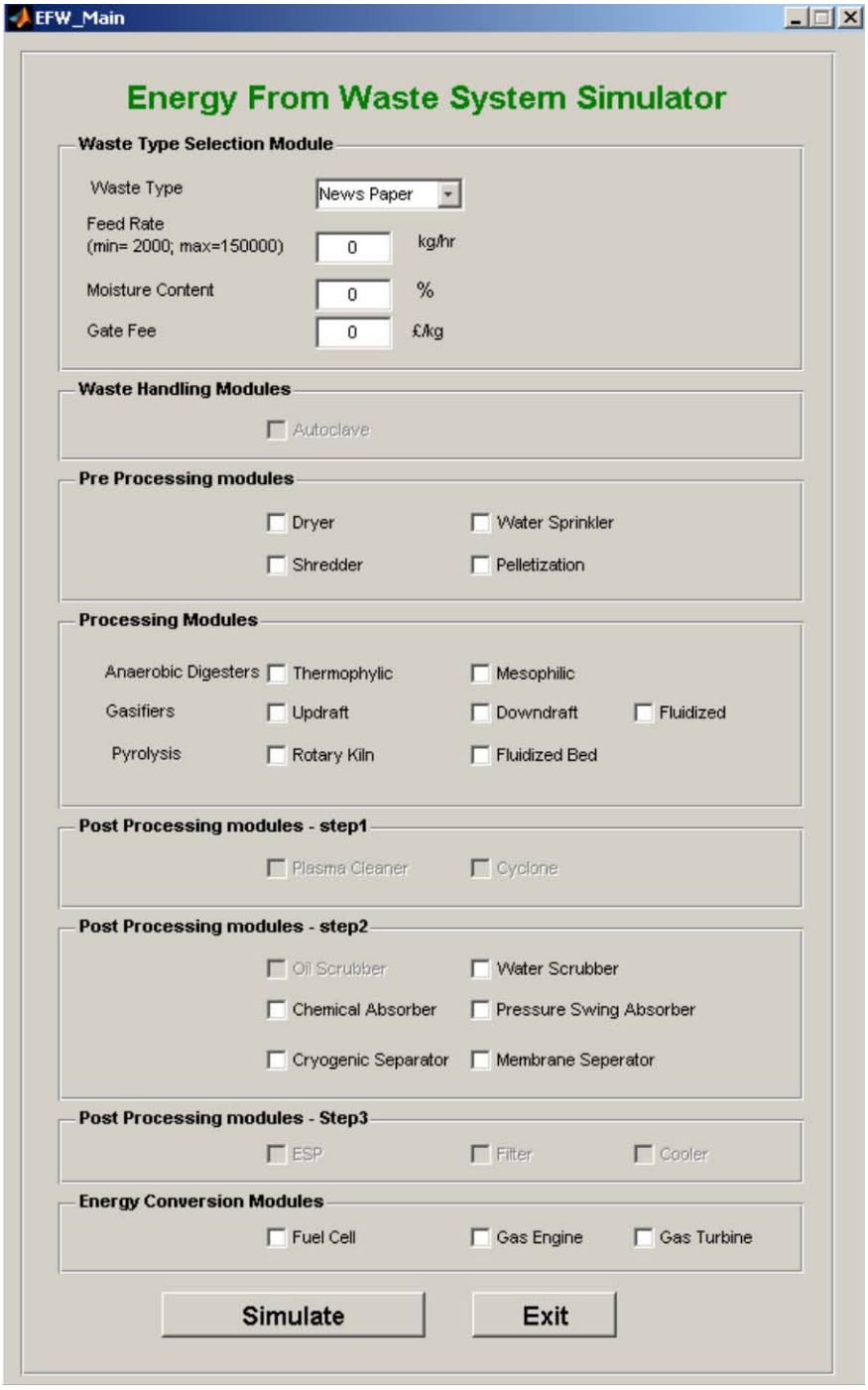


Figure 1 System Model GUI

Waste Type Selection

The main user defined input into the system model is the waste type to be simulated to be processed. The database of materials is currently focussed on common energy-bearing materials found in waste streams, in accordance with the scope of this project (waste sorting being out of scope). Glass is included as a sample material to illustrate the effect of inert materials in demanding process energy whilst not contributing on generation. Should there be a wish for further materials or capabilities to be incorporated into the model, the waste material database may be readily expanded in future versions of the model. The waste input into the system model is defined either for single materials, or for a mixed stream of the materials, illustrated in **Figure 2**. A pre-set mixture ratio for MSW is also included in the database, with the proportions based on the 2009 Resource Futures report as used in Work Package 1 of this project [3]. The waste sampling work in Work Package 1 illustrates the variability in waste streams, and the MSW mixture is not intended to be a definitive representation of UK MSW arisings, but rather an at-hand reference for users to draw on to compare the model outputs to other data sources. The term “Organic Fines” is used to encompass the wide variety of food waste materials which may be present in waste streams. The user defines the waste input for both single materials and the materials in a mix in units of kilograms per hour, thereby incorporating the proportional composition directly into the input data. Note that the throughput mass is the total, wet mass of the material, where its moisture content is separately defined. The selection interface for a mixed waste stream is shown in **Figure 3**. The user may also select the global material moisture content at this stage, as well as apply a gate fee (positive or negative), used to calculate the final cost of energy for the system.

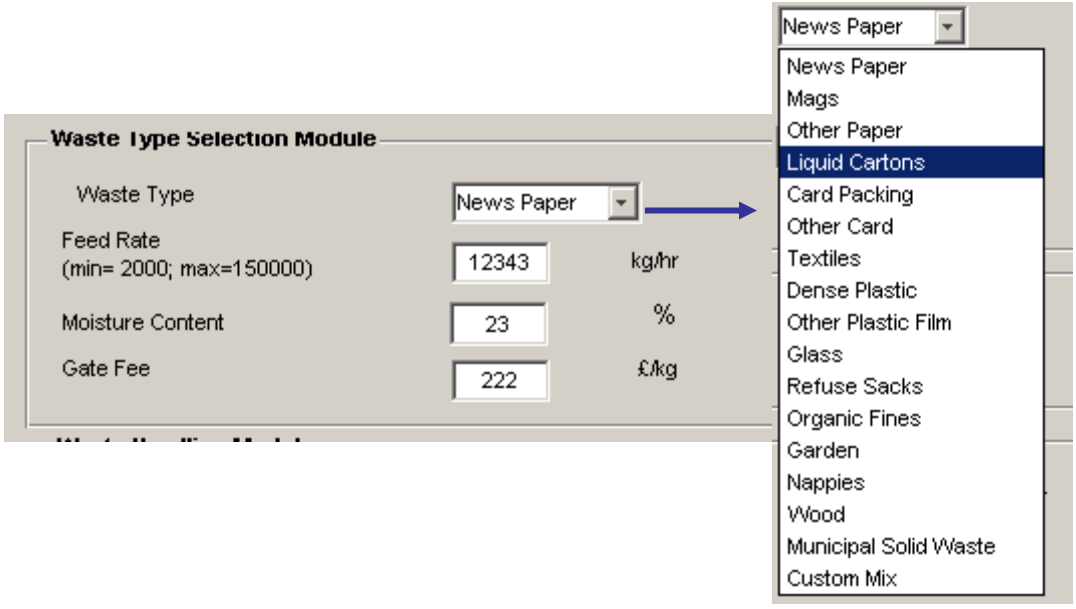


Figure 2 Waste Material Selection

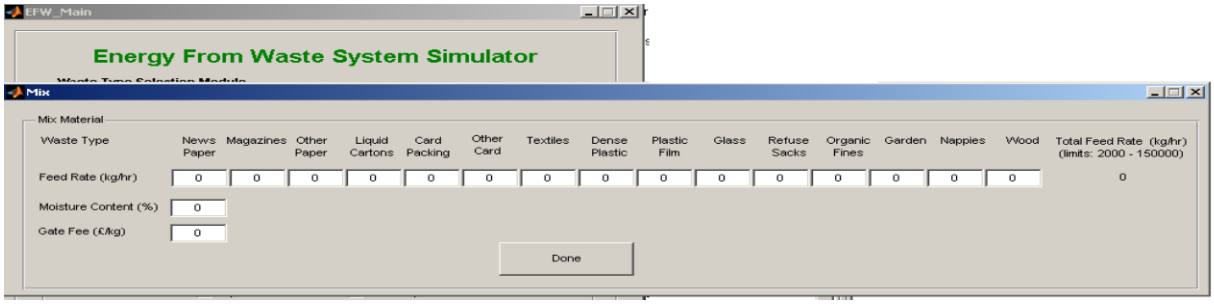


Figure 3 Mixed Waste Input Selection

Technology Selection

Following selection of the waste material, the user is able to select the technologies which may be considered by the model to comprise the final system by activating the check box next to each component technology. This feature was incorporated to enable model validation prior to the completion of all component models, and also for the potential use of the model in commercial applications, where technology options may be limited at any given time due to maintenance and repair etc.

Model Operation

When all available technologies have been selected, the “Simulate” button initiates the process simulations. Computation time is approximately 30 seconds per system (depending on computer capabilities), with a full factorial run (all technology options) taking about half an hour to run. Currently, there is no indicator for processing progress, although it is hoped to include this in a future version of the model. The user should ensure that no CSV files from previous runs of the model are open when starting the simulation mode, as this will corrupt the data files.

The results are generated in two CSV (comma separated variable) files, which can be opened with Microsoft Excel. These files are saved in the same directory as the model files. The `EfW_DOEResults.csv` file contains the details of each system (technology combination), and the gross and net thermal and electrical energy generated from the defined wastes. A second file, `EfW_DOEGasOutputs.csv` lists the gas composition as generated from the processor, and following post processing.

For model de-bugging, as well as for future interest, the outputs from each of the steps are saved as separate variables, and as such can be analysed following system simulation. As a final output, the model calculates the net electrical power and heat generated. For each system, the total capital and operational costs are also calculated.

Initial System Model Results

The system model has been developed to a state where it is functional, although as described above, further work is ongoing to validate assumptions in the models and check the model results. However, some indications of the current capabilities of the component and system models have been gained by running a number of scenarios. A general observation from a number of runs of the system model is that system requiring feedstock drying over a large moisture content differential often show a net thermal energy deficit. This may be representative of real world operation, where atmospheric drying would be largely used to dry material (not accounted for within the model),

although the model needs to be further examined to ensure the process heat outputs are accurately accounted for. In addition, the aspect ratio of a digester determines its surface area, and hence the heat loss to atmosphere. Consideration of this is currently contained within the anaerobic digester model, although a fixed aspect ratio of 4:1 (diameter:height) is assumed for all cases. A further iteration of the model may be made to incorporate an automatic optimisation of this aspect ratio to minimise reactor surface area and hence heat loss, which would be expected to have a material impact on the total system thermal energy balances.

As expected from the component model for the fixed bed gasifiers (up and down draft), care needs to be taken to ensure that negative values for the elements in the gas compositions and flow rates are not generated, leading to negative power generation values.

In addition, the updraft gasification model in particular appears to generated gases with a relatively high CO_2 and low H_2 content as shown in **Figure 4**. Experience from the tests conducted fro Work Package 2 and literature would suggest that further refinement of these models may be required, possibly based on a greater number of experimental conditions.

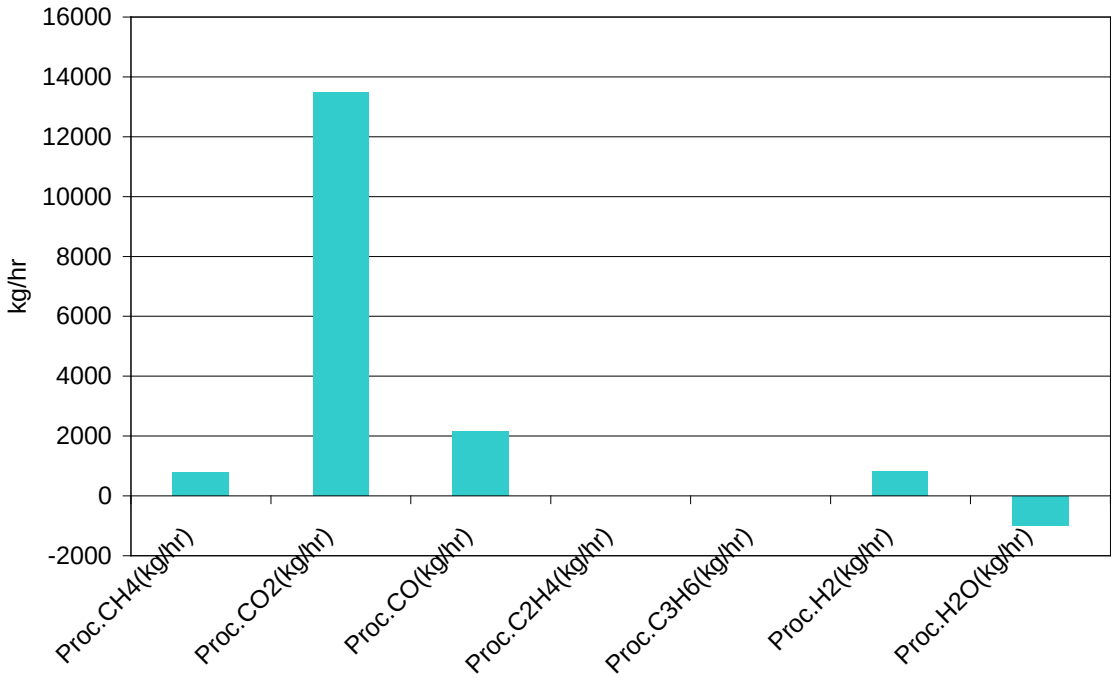


Figure 4 Example Gas Composition - Organic Fines, 56,000 kg/hr, Fluidised Bed Gasification

It has also been observed that the electrical power generation output from the systems incorporating a fuel cell appears remarkably high, whilst that of systems incorporating gas engines and turbines is considerably lower than might be expected. For example, the waste assessment conducted for Work Package 1 showed that the calorific value of typical waste materials is around 15 MJ/kg. As such, at a federate of 10000 kg/hr the energy input to the system is 150,000 MJ/hr, equating to 41 MW. At an expected average total system conversion efficiency of ~30% (current technology), the model

would be expected to indicate an electrical output of ~12.5 MW However, the model shows generated powers in the range of 1MW for this volume of federate when using a gas engine and turbine, and around 20 MW when using a fuel cell; the exact value depending on the material and system technologies. This is likely to be a result of the thermo chemical models over predicting the output of nitrogen and carbon dioxide based on the Work Package 2 test data. These inert gases are removed from the fuel stream in the reformer model inherent in the fuel cell model, resulting in a near pure stream of hydrogen. On the other hand, the high level of CO_2 would diminish the output of the combustion based generators.

In its current state the model does not incorporate any internal checks or requirements, and as such there are no cases which can not be operated. In reality, a number of constraints would be placed on technology combinations. For example, the gas flowing into a fuel cell would be required to be of a certain purity, with the limits on particulates, sulphur and other contaminants. The level of these inclusions in the gas would then determine whether the fuel cell would operate or not, and if so what the degradation rate would be (if any). These constraints are to be incorporated into the system model at the key interface points between the technologies at such a time when the model has been shown to operate robustly.

In the development of the scenarios from the project seminar, system models will be developed that will show how the technique operates. It is expected that when the consortium has developed the expected cases that waste to energy technologies will have potential the true capability of the tool will be seen. The outputs of all this proposed work will be shown in the 3.3 deliverable report.

Conclusions

The system model was produced to allow for an assessment of the economics of different technology configurations relative to the waste disposal and CO_2 emissions reductions relative to a baseline of mass burn incineration. Such an assessment was to indicate where technological developments could be made to decrease the cost of waste and emissions reductions, and to define system performance by process scale and hence population centre size. Whilst the final assessment of these benefits will be detailed in the benefits case which concludes this project (Work Package 4), the model under development is to enable appropriate data to be generated and explored.

To date, component technology models have been developed and integrated into a system level model to represent different configurations of end-to-end energy from waste systems. Initial assessment of the performance of the system model indicates that the system model functions appropriately, although with a number of discrepancies between the model outputs and expected values. Whilst such discrepancies are to be expected from a model undergoing development, the source for these discrepancies appears to be mainly the processor models. These have been developed based on the test data generated by Cranfield for this project. However, as described above, this data is discrete in nature, and as reflected at the Stage Gate 2 meeting of this project, requires further analysis and processing until it can be robustly incorporated into the models. In addition, further analysis of the test data is likely to indicate the benefits of further testing over a wider range of operating points for a single technology with a single material to assess the effect of the operating parameters on the technology outputs, and to ensure that these important relationships are accurately reflected in the models. A meeting is being scheduled between the modellers and experimenters for mid-August to assess the

data, and propose any further experiments which would add confidence and value to the model. A separate seminar has been scheduled for the consortium in mid-September to go through the model and explore the other variables and assumptions to further aid model robustness. The outcome of this seminar, alongside further model development will allow for the subsequent sensitivity analysis and variable optimisation planned for Deliverable 3.3 of this project.

For a definitive stratergy to be developed in the use of waste as an energy source the models and system models require more structured boundary conditions to be developed. The work performed at the seminar identifies the potential scenarios of location and scale that need to be investigated to recommend a series of technology options. Upon selection of the technology option there will be a need for further experimental work to develop a greater level of confidence in the products of the technology. There is a need for repeatability and reproducibility, even in such a varying feedstock such as waste.

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3. J. Parfitt, “Municipal Waste Composition, Trends and Futures”, Resourcefutures Report for Defra, April 2009
4. http://students.chem.tue.nl/ifp24/BiogasPosterWEB.pdf
5. www.water.org.uk

Appendix:

Molten Carbonate Fuel Cell Model Report

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Caterpillar Inc.: Jalaja Repalle

Abstract

The fuel cell model takes an input of mixed-hydrocarbon fuel gas together with oxygen from the air to form carbon dioxide, water, power and heat. The heat of reaction is used to maintain system temperature and reformer operation, hence once up to temperature the model requires no additional energy input. The model assumes that the fuel cell electricity generation process is 52.7% efficient. Excess heat produced is not used in this model. An overall mass balance is also presented.

Description

The model is based on the molten carbonate variety of fuel cell technology (MCFC). A molten carbonate fuel cell is an electrochemical system which converts hydrogen fuel gas into water, power and heat, without combustion.

The model is split into three main parts to represent the reformer operation, the cathode reaction and the anode reaction. In the reformer the hydrocarbon fuel is reacted with water to produce CO_2 and H_2. The reformer output then passes into the anode compartment. At the cathode side, oxygen from the air and carbon dioxide recycled from the anode exhaust react with the addition of 2 electrons from the electrical circuit to form a CO_3^{2-} carbonate ion. This carbonate ion passes through the molten carbonate electrolyte to the anode side where it reacts with the hydrogen fuel to form water, carbon dioxide, power and heat. Air in excess to the stoichiometric requirements is used.

In order for the MCFC to function, it is necessary to operate it at a temperature in the region of 902-983K. Initially this heat must be provided from an external source, such as electricity or a gas burner. Once the fuel cell is up to temperature, the heat of reaction is sufficient to maintain its operating temperature.

Assumptions

- It is assumed that the system is at temperature and that no additional heat is required. No allowance is made for energy required to raise the system to temperature initially. If the system operating temperature goes beyond the accepted range (902-983K) then the fuel cell operation is assumed to cease.

- It was assumed that all hydrocarbons that were steam reformed would also undertake the gas-shift reaction, converting CO and H_2O to CO_2 and H_2.
- The steam to fuel carbon content ratio is always assumed to be sufficient to convert all the hydrocarbon fuel supplied (suggested between 2 and 3).
- The system is assumed to be 41% thermally efficient with regard to usable heat (that is 41% of electrical output), with the remaining energy being lost to the environment.
- Assumed that the composition of air is 78% N_2 and 22% O_2
- It is assumed that the exhaust gas from the anode is mixed with air and entered into the cathode to provide sufficient O_2 and CO_2.
- The effect of the contaminants on system performance has been difficult to quantify. Therefore a performance degradation of 1% for every 100% a contaminant is over the threshold limit was assumed.
- Stack degradation also leads to system performance loss so it was assumed based on the literature that 1% of system performance would be lost for every 1000 hours operation for the first 16,000 hours. After this period there would be 4% of system performance loss for ever 1000 hours operation.

Inputs/Outputs

Input Parameters		Units
Reformer input		
	Gas Flow	Kg/hr
	Gas composition	Wt % of mixture of various hydrocarbons
Operating Conditions		
	Stack run time	Hours
	Hydrocarbon conversion	%
	Steam to carbon ratio	
	Hydrogen utilisation	%
	Inverter efficiency	%
	Input gas temperature	K
	Input gas pressure	Bar
	Operating pressure	Bar
	Specific heat of gas	J kg^{-1} K^{-1}
	Compressor efficiency	%
	Operating Temperature	K
	Optimal system electrical efficiency	%
	Contaminant levels	Ppm (H_2S, NO_x, HCl, particulates (>3μm), alkaline metals) % NH_3

Validation

The model was validated and judged to be acceptable.

References

- Wolf Vielstich, Arnold Lamm, Hubert A. Gasteiger
  “Handbook of Fuel Cells – Volume 4 – Fundamentals, Technology and Applications”
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- F Orecchini, E. Bocci, A. Di Carlo: MCFC and Microturbine power plant simulation, Journal of Power sources, 160 (2006) 835-841
- James Larminie, Andrew Dicks: Fuel Cell Systems Explained, 2nd Edition, Wiley

Glossary

- **MCFC:** Molten Carbonate Fuel Cell.
- **Cathode:** Electrically positive electrode which air is applied to.
- **Anode:** Electrically negative electrode which fuel (hydrogen) is applied to.
- **Electrolyte:** Molten mixture of alkali metal carbonates which is electrically isolating but conducts carbonate ions when at temperature.
- **Reformer:** A system which catalytically converts hydrocarbon gases into hydrogen rich fuel stream and carbon oxides (CO & CO_2).