A Multidimensional Model of Direct-Steam Heating of Newspaper and Municipal Solid Waste in a Hydrothermal Reactor

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The use of high pressure steam is one of the options that is under consideration as a means of heating raw MSW to temperatures at which sufficient hydrothermal decomposition will occur to allow a high solid content slurry to be produced. This slurry could potentially be used as a feedstock to gasifier which in turn would produce syngas. The required temperatures and pressures to allow the hydrothermal decomposition reactions to proceed are in the range of 275-350 C and 6-18 MPa. In two recent reports the steam heat option was explored for a proposed pilot scale operation¹ and for a conceptual commercial scale operation². The reported work centered around the use of computer models to simulate the process. In both cases the models used did not address the spatially resolved details of the processes occurring inside the actual high pressure reactor vessels.

In the conceptual commercial scale model, the ASPEN PLUS process simulator was used to simulate the important processes. ASPEN PLUS is primarily a steady-state simulator and consequently the batch processes involved in steam heating of MSW were simulated by continuous process modules. This allowed overall material and energy balances to be performed but did not deal directly with the transient nature of the processing.

In the pilot scale modeling, a transient model was developed to look at processing options using currently available pilot equipment. Although transient, the model did not deal with the details of what was occurring inside the reactor vessel.

This report describes a general purpose packed bed model originally developed for gasification modeling³, which has been modified to a form that can address some aspects of the steam heating which occurs inside a hydrothermal reactor vessel. The multidimensional model solves energy and mass conservation equations for a packed bed system containing gas and solid phases. It can solve one dimensional, two dimensional and axisymmetric three dimensional problems. The solid phase is assumed to be stationary and the gas phase velocity field is assumed to be governed by Darcy's law. The model formulation allows multiple solid and gas species to be defined. Generalized reactions involving all defined species can be easily incorporated into the model. A variety of boundary conditions, including time dependent conditions, can be specified. For the steam heating application, one of the solid species was recast to be water. A suitable reaction describing condensation and evaporation of water was formulated. In addition, equations were added to the model which allows the temperature of the reactor wall to be computed along with the solution for the interior.

The reformulated model is capable of doing computations on the systems of interest as long as the water phase is assumed to be basically immobile. The severity of this limitation is difficult to gauge. In general, systems of interest consist of porous particles. The porous particles, paper or other biomass derived constituents, have a network of small pores which effectively can immobilize large quantities of water by capillary action. The true physics of water flow in such systems is in general very complicated because of the presence of a variety of materials, discrete particles, varying

water saturations and changing physical character of the solid matrix. Consequently, the behavior a system with no water flow is both a tractable and useful limiting case.

Below the equation set used in the model and related physical and chemical submodels are described. Following this results are presented for model calculation related to a pilot scale system and to a conceptual commercial scale operation.

THE MODEL

The primary model equations are the conservation equations for solids, gases and energy in a packed bed. The following assumptions are implicit in the formulation - used:

- Temperatures of gas and solid phases at a given point are equal
- The gas phase follows the ideal gas law
- Gas flows according to Darcy's Law
- The geometry of the bed is assumed to be one dimensional, two dimensional rectangular, or two dimensional axisymmetric.
- Liquid water is assumed immobile
- The bed is in contact with solid walls at the bottom and the sides, no wall is present at the top of the bed

The model treats solid and gas species. Since liquid water is not allowed to move it is treated from the model's standpoint as a solid. The current model includes:

- Four solid species
 - Ash - inert
 - Water - immobile liquid water
 - ORG - organic material which undergoes decomposition
 - GORG - solid product of decomposition
- Eight gas species are defined
 - nitrogen
 - oxygen
 - hydrogen
 - carbon monoxide
 - carbon dioxide
 - water vapor
 - methane

The model can easily accommodate inclusion of additional gas or solid species.

Conservation Equations

The overall gas phase conservation equation for the system is

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A MULTIDIMENSIONAL MODEL OF DIRECT-STEAM HEATING OF NEWSPAPER AND MUNICIPAL SOLID WASTE IN A HYDROTHERMAL REACTOR

C.B. Thorsness

Abstract

Hydrothermal treatment (reaction in a water medium at elevated temperatures) can transform many municipal solid waste (MSW) constituents into a synthetic coal material which is more amenable for use as a fuel or chemical feedstock than the raw MSW. One means of heating the MSW is to use direct high temperature steam injection into a closed reactor and allow the latent heat of the steam to raise the MSW to the desired temperature and at the same time build the pressure necessary to maintain a water phase. This report describes a computer model which can be used to look at details of the steam flow, water evaporation/condensation, thermal evolution, and MSW decomposition in a direct-steam heated MSW hydrothermal reactor. The model treats the system as a packed bed using a Darcy's law formulation for computing gas flow rates. The model has been applied to a pilot and a commercial scale system. Computations take between 1-6 hours on a HP-9000/730. Initial computations performed with the model indicate that pressure drop and velocities on a pilot scale systems will be small. On the other hand, they indicate that gas velocities inside a commercial scale reactor can reach levels at which entrainment of liquid or solids could occur. In addition, on the commercial scale, model results indicate that in the absence of liquid water flow the thermal coupling between vessel contents and heavy reactor walls should be small thus minimizing unwanted heat loss.

INTRODUCTION

Municipal solid waste (MSW) represents a largely untapped domestic energy source of considerable magnitude. Two major difficulties in utilizing the resource is its high water content and its physical heterogeneity. One approach to overcoming these problems is to develop pretreatment processes which produce a more conventional fuel product. Hydrothermal treatment, the use of hot water at elevated temperatures and pressures, is one way of accomplishing this task. Hydrothermally treated MSW forms a concentrated water slurry very much like conventional coal water slurries. This slurry can be used to feed conventional processing equipment, such as a gasifier, in order to convert it to high value products.

$$\frac{\partial(\phi C)}{\partial t} = -\bar{\nabla} \cdot (\bar{v} \phi C) + \sum_{i=1}^{i=n} Q_i + \sum_{i=1}^{i=n} s_i ,$$

where C is the total gas molar concentration in mol/m³ of gas filled porosity, ϕ is the total bed porosity, t is time, v is the effective gas velocity, Q_i is the rate of introduction of gas species i into the bed, s_i is the source rate of species i per unit volume of bed from reaction, and n is the number of gas species defined for the problem. The overbar indicates a vector quantity.

The effective gas velocity, v , as used here is related to the superficial (or darcy) velocity and the interstitial velocities in the following way. The superficial velocity is a convenient measure of how gas is flowing through a multiphase system, it is based on the total area of the system. The superficial velocity times the cross sectional area gives the total volumetric flow rate. In the present formulation there is assumed to be porosity present both external and internal to particles making up the bed. The effective velocity is the velocity which gives the proper flow when the cross sectional area is multiplied by the total porosity. The interstitial gas velocity, on the other hand, is defined such that its product with the external porosity and cross sectional area yields the total volumetric flow rate. It is equal to the true average gas velocity if all gas flow is through the external porosity. The three velocities are related by

$$U = \phi_e v_{\text{int}} = \phi v ,$$

where U is the superficial velocity, ϕ_e is the porosity external to the particles, and v_{int} is the interstitial velocity.

The model uses a conservation equation for each gas species. These equations have the form

$$\frac{\partial(\phi c_i)}{\partial t} = -\bar{\nabla} \cdot (\bar{v} \phi c_i) + Q_i + s_i + \bar{\nabla} \cdot (C \bar{\bar{D}} \cdot \bar{\nabla} y_i) ,$$

where c_i is the concentration of gas species i in mol/m³ of gas filled porosity, D is the effective mass dispersion in the bed, and y_i is the mole fraction of gas species i . The double overbar denotes a tensor quantity.

Similarly there is an equation describing the conservation of each solid species. This equation includes only two terms since the solids are assumed stationary. Each equation is of the form

$$\frac{\partial \rho_k}{\partial t} = s_k^* ,$$

where ρ_k is the effective density of solid species k defined as mass per total unit volume of the system, and s_k^* is the solid source term for solid k .

The final conservation equation for the system is that for enthalpy

$$\frac{\partial \left[\phi \sum_{i=1}^{i=n} (c_i h_i) + \sum_{k=1}^{k=m} \rho_k h_k^* \right]}{\partial t} = -\bar{\nabla} \cdot \left[\sum_{i=1}^{i=n} (\bar{j}_i h_i) \right] + W + \bar{\nabla} \cdot (\bar{k} \cdot \bar{\nabla} T),$$

where h_i is the enthalpy of gas species i , h_k^* is the enthalpy of solid species k , j_i is the flux of gas species i , W is local heat source strength, and k is the effective thermal conductivity.

These conservation equations represent the time dependent equations solved by the model. For a system with four solid species and seven gas species a total of 12 equations are defined. The apparent redundancy of the overall gas conservation equation and the individual gas species equations is removed when it is recognized that the independent variable pressure does not appear explicitly in the above conservation equations. Adding pressure to the other 11 dependent variables (gas and solid species concentrations and temperature) yields 12 dependent variables.

Gas Species Flux

The flux of each gas species, j_i , is computed using the following

$$\bar{j}_i = \bar{v} \phi c_i - \bar{D} \cdot (C \bar{\nabla} y_i).$$

Because this is only an approximate formulation of the true gas species flux within the system and because the effective dispersion coefficient, D , is obtained from an approximate model, only the diagonal components of the dispersion tensor are retained.

The dispersion coefficient is obtained from correlations available in the literature for axial and perpendicular dispersion in packed beds. The axial and perpendicular directions are defined in terms of the direction of gas flow. For the perpendicular component, that component acting perpendicular to the direction of gas flow, a correlation due to Bischoff⁴ is used

$$D_p = D_g (0.73 \phi_e + 0.1 Re Sc),$$

where D_g is the molecular diffusivity, Re is the particle Reynolds number, Sc is the Schmidt number. The Reynolds number is defined by

$$Re = \frac{\rho_g d_p U}{\mu},$$

where ρ_g and μ are the gas density and viscosity respectively. The axial component is obtained from a correlation of Edwards and Richardson⁵

$$D_a = D_s \left[0.73\phi_e + \frac{0.5(\text{Re}Sc)^2}{9.7\phi_e + \text{Re}Sc} \right].$$

From these components and the appropriate direction cosines the diagonal terms of the dispersion tensor are computed.

Gas Velocities

Gas velocities are computed assuming Darcy's law holds. Darcy's law is generalized to the following

$$\bar{U} = \frac{\bar{\Gamma}}{\mu} \cdot \bar{\nabla} P,$$

where Γ is the permeability of the bed. Only the diagonal elements of the permeability tensor are retained. The permeability is assumed to be a function of the local external porosity using the simple relation

$$\begin{aligned} \Gamma_{jj} &= \Gamma_{jj}^{\circ} \left[\gamma_i + (\alpha - \alpha_i) \frac{\gamma_h - \gamma_i}{\alpha_h - \alpha_i} \right] \text{ for } \alpha_h < \alpha < \alpha_i, \\ \Gamma_{jj} &= \Gamma_{jj}^{\circ} \gamma_h \text{ for } \alpha_h \geq \alpha, \text{ and} \\ \Gamma_{jj} &= \Gamma_{jj}^{\circ} \gamma_i \text{ for } \alpha \leq \alpha_i. \end{aligned}$$

Here, α represents a pseudosaturation defined by

$$\alpha = \frac{\phi_e}{\phi_e^{\circ}},$$

where ϕ_e° is the initial external porosity. The jj subscript stands for either of the diagonal elements of the permeability tensor. Γ_{jj}° is the initial value of absolute permeability ($\phi_e = \phi_e^{\circ}$ and $\gamma_i = 1$). The method of computing the current external porosity is described in a later section. This very simplistic relative permeability model simply allows the permeability of the bed to be reduced when the external porosity begins to be filled by water.

Bed Thermal Dispersion

Like the effective mass dispersion the effective bed thermal dispersion is obtained from correlations available in the literature for axial and perpendicular thermal dispersion, conductivity, in packed beds. Again, for reasons equivalent to those given for mass dispersion only the diagonal components are retained. The axial and perpendicular directions are defined in terms of the direction of gas flow. Both components are obtained from the work of Wakao and Kaguei⁶. For the perpendicular component, that component acting perpendicular to the direction of gas flow, the correlation used is

$$k_p = k_g (k_0 + 0.1 \text{Re} Sc),$$

where k_g is the conductivity of the gas phase and k_0 is the conductivity of the bed with no flow. The axial component is given by

$$k_a = k_g [k_0 + 0.5 \text{Re} \text{Pr}].$$

From these components and the appropriate direction cosines the diagonal terms of the thermal dispersion tensor are computed.

The effective conductivity at no flow, which includes a radiation contribution, is given by the same workers as

$$k_0 = k_g \left[\phi_s Nu_v + \frac{1 - \phi_s}{\frac{k_g}{k_p} + \frac{1}{25 + Nu_s}} \right],$$

where k_p is the conductivity of the solid particles. The so called Nusselt numbers for the solid and gas used in this correlation are given by

$$Nu_v = \frac{d_p}{k_g} \left[\frac{0.2268 \left(\frac{T}{100} \right)^3}{1 + \left(\frac{\phi_s}{1 - \phi_s} \right) \left(\frac{\varepsilon}{2 - \varepsilon} \right)} \right] \text{ and}$$

$$Nu_s = \frac{d_p}{k_g} \left[\frac{0.2268 \left(\frac{T}{100} \right)^3}{\frac{\varepsilon}{2 - \varepsilon}} \right],$$

where ε is the emissivity.

In the Wakao and Kaguei model the particle conductivity k_p is assumed known. Within the conceptual model used here, the particle themselves are assumed to be composed of solid and void and therefore it may not be appropriate to use the solid conductivity, as is called for in the Wakao and Kaguei model, for the particle conductivity. Instead, the particle conductivity is estimated by reapplying the above three equations to the particle itself assuming no flow. To do this the porosity internal to the particle replaces the external porosity and a new effective particle size replaces the bed particle size. The particle size is a length scale which characterizes the porosity of the system. In the current model the particle size used in the model for the particle conductivity has simply been set to one tenth of the particle size chosen for the bed. Since the conductivity model does not equal the solid conductivity at zero porosity the relation has been modified to force it to do so at low porosity. The following has been used

$$k'_s = k_s(1 + 20\phi_{int}) \text{ and } k'_s \leq k_s \text{ for } \phi_{int} < 0.1,$$

where the k'_s is the modified particle conductivity, k_s is the solid conductivity, and ϕ_{int} is the porosity of the particle. A similar modification to the overall no flow bed conductivity is made at low external porosities.

Gas Properties

Thermodynamic and transport properties for gas species are required to solve the models conservation and transport equations. In some cases the property is defined for an individual gas species and in others an average value for the gas mixture has been used. In most cases the parameters defining the properties are input parameters to the model.

Those properties which are used for the gas mixture and for individual species as need include heat capacity, viscosity, Prandtl number and Schmidt number. The gas heat capacity is defined for all gases using a three term polynomial in temperature

$$c_g = c_{g0} + c_{g1}T + c_{g2}T^2.$$

The viscosity is defined using a linear function in temperature

$$\mu = \mu_0 + \mu_1T.$$

The Prandlt number and Schmidt number

$$\text{Pr} = \frac{c_g \mu}{k_g},$$
$$\text{Sc} = \frac{\mu}{\rho_g D_g},$$

are assumed to be constants.

Finally, each gas species is assumed to have a specific molecular weight and heat of formation.

Solid Properties

The required solid properties include density, heat capacity, and heat of formation. Each solid species is assumed to have an intrinsic density. This density is used to compute required system porosities using the following relations

$$\phi = \sum_{k=1}^{k=m} \frac{\rho_k}{\rho_{k_s}},$$

where ρ_{k_s} is the intrinsic density of solid species k . Other porosities are defined in terms of this value. Increases or decreases in porosity are assumed to occur first within the particles. In the case of a decrease in porosity, due for instance to water condensation, it is assumed that once the internal particle porosity is filled the external porosity is decreased to reflect further filling of void space.

A heat capacity and heat of formation is defined for each solid species. The individual heat capacities are assumed functions of temperature through the use of a second order polynomial in temperature.

A single solid thermal conductivity and solid emissivity is assumed. The conductivity is assumed to be a linear function of temperature, while a constant value is used for the emissivity.

Boundary Conditions

The model is able to accommodate a variety of boundary conditions. A number of boundary conditions can be prescribed functions of time. The boundary conditions are applied at four locations, the inlet plane at $y=0$, the exit plane at $y=L$, the centerline at $x=0$, and the wall. Here, the y -dimension is measured from inlet plane to outlet plane. For the one-dimensional case it is the only dimension. The x -dimension is used as the coordinate perpendicular to the y -direction and is either a linear dimension in a two-

dimensional rectangular problem or the radial dimension in an axisymmetric three dimensional calculation.

At the inlet plane the gas species flux (gas injection rate) is specified as a function of time and the thermal boundary condition is imposed using

$$\sum_{i=1}^{i=n} f_i h_i = \sum_{i=1}^{i=n} j_i h_i - k \frac{\partial T}{\partial y},$$

where f_i is the prescribed injection flux of gas species i and the temperature derivative is evaluated at $y=0$. These boundary conditions are applied at each part of the boundary where gas is injected. The model allows gas injection to occur over all or a part of the $y=0$ boundary. For those parts of the $y=0$ boundary for which gas is not injected boundary conditions equivalent to those applied to the wall, $x=R$, can be applied.

At the exit plane, $y=L$, gas leaves the system and a zero gradient is imposed on the gas species concentration and temperature. The rate of gas flux out of the system, G , is set using

$$G = \frac{\beta \Gamma}{\mu} (P - P_o) \quad \text{for } P > P_o, \text{ and}$$

$$G = 0 \quad \text{for } P \leq P_o.$$

Here, P_o is the outlet sink pressure which may be a function of time, and β is a parameter. For large values of β this formulation basically sets the pressure at the outlet plane to the prescribed value. However, a compromise is needed between imposing the desired pressure at the outlet plane and computational difficulties.

Consequently, β is chosen large enough to have P essentially equal to P_o at the outlet plane but small enough so that the solution of the model equations does not become too difficult.

At the centerline the gradient of all dependent variables are set to zero.

At the wall, $x=R$, and along the noninjection $y=0$ plane boundary conditions for gas species concentrations, total gas concentration and temperature are required. Since the wall represents a no flow boundary gradients of gas concentration are set to zero, this in turn dictates a zero gas velocity in the direction perpendicular to the wall.

The thermal boundary conditions at the wall are more complicated because adiabatic and nonadiabatic conditions are modeled. For the adiabatic condition the temperature gradient perpendicular to the wall is set to zero. However, for systems in which heat is transferred from the bed to the wall continuity of heat flux is imposed by

$$\frac{\partial T}{\partial \eta} = \frac{h_w (T - T_w)}{k},$$

where η is the direction perpendicular to the wall, h_w is the wall heat transfer coefficient, and T_w is the wall temperature. The model allows the wall temperature to be set at a constant value or to be a function of time based on the solution to a simple wall model described in the next section.

Wall Model

The bed is assumed to be enclosed by vessel walls at the bottom and sides. The top of the bed is assumed not to be in intimate contact with the vessel top. The overall model includes a submodel for the time evolution of the temperature of the enclosing walls which is in the form of an energy conservation equation for the wall

$$\frac{\partial T_w}{\partial t} = \frac{h_w(T - T_w) - h_\infty(T_w - T_\infty) + l_w q_w}{l_w \rho_w c_w},$$

where h_∞ is the heat transfer coefficient between the wall and the surroundings, T_∞ is the temperature of the surroundings, l_w is the thickness of the wall, ρ_w is the density of the wall, c_w is the heat capacity of the wall, and q_w is a heat generation rate in the wall. This formulation allows the temperature of the wall of the enclosing vessel to be computed as a function of time. It allows for energy exchange with the interior and exterior as well as the simulation of wall heating, for instance by electrical wall heaters. The model formulation allows h_∞ and q_w to be specified functions of time.

The wall to bed heat transfer coefficient can either be given a set value or it can be computed using a correlation for wall heat transfer in packed beds. The computed wall heat transfer coefficient (Yagi and Wakao⁷) is given by

$$\begin{aligned} h_w &= \frac{0.2k_g \text{Re}^{0.8} \text{Pr}^{1/3}}{d_p} \quad \text{for } \text{Re} > 40, \\ h_w &= \frac{0.6k_g \text{Re}^{0.5} \text{Pr}^{1/3}}{d_p} \quad \text{for } 1 < \text{Re} \leq 40, \\ h_w &= \frac{0.6k_g \text{Pr}^{1/3}}{d_p} \quad \text{for } 1 \leq \text{Re}. \end{aligned}$$

Here, Re is the Reynolds number for the particles previously defined. The last relation is not from the original correlation but has been added so that some conductivity is maintained as the flow rate gets small.

Reactions

Only two reactions are defined in the model, although it is a straightforward matter to add more as needed. The two reactions are steam/water evaporation/condensation and decomposition of solid species ORG to GORG.

The decomposition reaction is handled as a simple first order decomposition with an Arrhenius rate constant.

$$k_r = A \exp\left(\frac{-T_a}{T}\right)$$

The products are assumed to be a solid, GORG, water, and carbon dioxide, hydrogen and methane.

The use of a rate expression for evaporation/condensation of water was not done because the actual kinetic rate is considered an important phenomena to incorporate into the model. To a very good approximation the distribution of water between the liquid and vapor phase is dictated by equilibrium considerations. However, the model formulates all species changes as a rate process. To deal with an equilibrium process in an explicit manner would require a complete reformulation. Besides, for sufficiently rapid evaporation/condensation rates formulated with the appropriate driving force the rate based system results in computed systems in which there is essentially an equilibrium relation between the water vapor in the gas phase and the liquid water. The following is the reaction rate currently defined in the model for evaporation/condensation

$$r_w = \sigma [10 D_g d_p] V_p (c_e - c_{H2O}).$$

The rate is expressed per unit volume of bed. The term in parenthesis is the concentration driving force which can result in either a positive rate, evaporation, or a negative rate, condensation. The term in square brackets just allows some scaling based on a diffusional type resistance. V_p is the particle number density (number of particles per unit volume of bed), c_e is the concentration of water vapor at saturation for a given temperature, c_{H2O} is the concentration of water vapor, and σ is a scaling factor which can be selected to scale the rate for a particular problem. In general σ should be selected to be as large as possible without causing undue computational difficulty.

Two modifications are made to this basic rate expression to handling limiting cases. When the driving force results in evaporation and the amount of liquid water present is low the rate of evaporation is reduced by the square of effective liquid water density for values of the effective water density less than 1 kg/m^3 . This allows the rate to be smoothly reduced as the solid dries out. Another limit is needed to handle the case when all the void space is filled. Thus for a situation in which condensation is occurring the rate is multiplied by the total porosity thus reducing the rate to zero as the porosity is filled.

The computer code which embodies the solution scheme is quite flexible. A variety of boundary conditions, initial conditions, geometry and problem physics can be specified

quantities. Details of the differencing scheme used are available in reference 3. auxiliary calculations required for the solution, e.g. transport and thermodynamic values. Large negative values of dependent variables can result in a breakdown of in which no solution is possible because of the generation of large nonphysical negative by increasing numerical dispersion, but large spatial oscillations can lead to situations formation of spatial oscillations of convected quantities. This compromises the accuracy upwind, or donor cell differencing, of convective terms was used to protect against the Wherever possible the conservative nature of the equations was preserved. Also In developing the discretized equations standard finite difference methods were used.

nodes in the x-direction (second linear or radial dimension). number of dependent variables selected for a given problem as well as the number of the solution of the stiff equation set. The bandwidth of the problem is related to the option method 25 is used. This option uses an internally generated banded Jacobian in number of optional methods to be used in solving systems of ode's. In this case the computer model which solves the model equations. LSODE provides the user with a developed at LLNL by Hindmarsh⁸, is such a solver and has been incorporated into the handling stiff systems of equations. LSODE, a widely available software packaged power of the method stems primarily from choosing a robust ode solver capable of used to integrate the system of equations in time to yield the required results. The yields a set of ode's with time as the independent variable. A suitable ode solver is then differential equations (pde's) by discretizing the pde's in the spatial dimensions. This differential equations (ode's). These ode's are obtained from the model partial The Method of Lines scheme is based on the solution of a set of initial value ordinary making use of a Method of Lines solution scheme. This solution scheme was originally chosen because of the flexibility it offers in formulating the physics of a problem. The method also handles 1, 2 or 3 dimensional problems in a straightforward manner.

Solution Scheme

where the pressure is given in MPa.

$$P_w = 8.8888 \times 10^4 \exp\left(\frac{-5114.6}{T}\right) \text{ for } T < 410.57K, \text{ and}$$

$$P_w = 2.9829 \times 10^4 \exp\left(\frac{-5114.6}{T}\right) \text{ for } T \geq 410.57K.$$

pressure of water

The saturation condition is computed using the following correlation for the vapor

through input data. This includes the ability to select a subset of gases to be considered from the list of seven gas species currently available in the model. For problems in which the important physics can be captured with only a few gases, this feature can greatly improve solution efficiency and thus running time. The code is modular enough to allow the addition of new gas and solid species and additional reactions. The code is designed so that a given problem can be repeatedly restarted from any desired point in its evolution and new problem parameters can be specified. This can greatly reduce the computational effort in doing parameter studies as well as provide a means to recover from minor computing problems that may arise.

One problem, not addressed in the original model, encountered in using the model for the hydrothermal processing is the loss of accuracy of flow related terms associated with large changes in pressure. In the original gasification related use of the model the pressure of the system tended to not change greatly during a simulation. However, in the hydrothermal processing case a change of 100 fold in the average system pressure during a simulation is routine. The large pressure change causes a problem in the following manner. For a given problem the magnitude of gas flows on a mole basis tends to be of the same order during all phases of the operation. This means that for a fixed bed permeability pressure drops caused by the flows may be easily resolved at low pressures but at high pressures the same flow results in pressure drops which are a much smaller fraction of the average pressure. This can lead to numerical difficulty if the pressure drop to pressure ratios fall to the level of the typical numerical error control, 10^{-4} to 10^{-5} .

One way to overcome this problem would be to reformulate the problem using an isobaric assumption within the system. Gas flows would then be computed based on mass balances alone. This solution was rejected, at least for now, for two reasons. First this would require a substantial rewrite of the computer code which would obviate part of the motivation for using an existing code for the current work. Secondly, it is probable that pressure drop limitations within the bed will be important in limiting operating flow rates during part of the process cycle. Consequently, the ability to compute these pressure drops is useful.

The approach taken to deal with the problem was to allow the bed permeability to be changed as a function of the state of the process, particularly its pressure. This change is nonphysical, in that it is done to allow the solution of the model equations and not because of a true change in bed permeability. It does, however, allow actual pressure drops to be computed during low, pressure operations when they are important. As pressures increase and the accuracy of computed flow rates becomes a problem the permeability of the bed is artificially increased to increase the size of the computed pressure drops and the accuracy of the flow rates based on them. As pressures decrease, the permeability is increased again to allow calculation of true pressure drops at low pressures.

The computer model currently provides two means of permeability control. The first is a simple provision for switching from the true bed permeability to an artificial

permeability for high pressure calculations. Preliminary tests, indicated this could work but it was very tedious to tailor the amount of permeability change and the pressure level at which the change is made for a particular problem. As a result, a second option was implemented which allowed the permeability to be automatically scaled as average pressure drop in the system changed. This allows adequate accuracy to be maintained to complete the calculations even though average system pressures change by orders of magnitude during a single run. Further comments on the viability and suitability of this scheme is made in later sections dealing with computed results.

Pilot Scale System

The model has been applied to a pilot scale hydrothermal operation. The system of interest is a pilot scale reactor vessel which is approximately cylindrical, 1.3 m in diameter and 1 m high. It is filled with damp newspaper which is to be heated by introduction of high pressure steam. The initial condition of the system is assumed to be the filled vessel with an effective newspaper density of 180 kg/m^3 (204 kg total) and an effective water density of 90 kg/m^3 (102 kg total). The porosity is assumed to be initially air filled, the pressure is assumed to be 0.1 MPa and the temperature of contents and walls is taken as 25 C.

The need to start with damp newspaper to insure adequate water saturations during the reaction phase was based on previous work¹. The operating time line was also developed based on previous model results described in reference 1. The planned operation of the pilot reactor calls for heating the vessel walls, which are 3.8 cm thick steel, to 150 C with external heaters available on the pilot unit. During this period it is anticipated that heat transfer to the interior will be limited by the development of a dry layer near the wall. Then saturated steam at rates up to 2 mol/s are to be injected into the bottom center of the reactor for 145 minutes. During this operation the dry wall layer should resaturate, additional water will condense. Overall system temperatures and pressures will increase until they reached the desired 6.3 MPa and 280 C. Following this the steam flow is to be reduced to 0.5 mol/s for 30 minutes. This completes the heatup and reaction phase. Next the steam is to be shut off and the pressure reduced to atmospheric over the course of 100 minutes. At this point the contents of the vessel will be at 100 C and a dry layer will probably have reformed at the wall due to the large heat capacity of the metal walls. Since handling the product at this temperature may be difficult, particularly for the first run, the system will need to cool further. This cooling will be accomplished only by conduction from the vessel which is covered by a 10 cm of insulation and consequently will take several days to complete.

Model parameters used in the simulating this sequence of operations are listed in Table 1. The wall heat transfer coefficient, h_w , was held constant and chosen to be large enough so that the computational cell immediately adjacent to the wall is strongly coupled to the wall temperature. As a result the transport near the wall is modeled by the fundamental equations for the packed bed and consequently a relatively fine mesh

is needed near the wall. The wall region was handled in this way because condensation and evaporation near the wall caused by the metal vessel walls make the use of the general wall model inappropriate.

Table 1. Model parameters used in pilot scale calculations.

Parameter	Value	Parameter	Value
h_w (W/m ² -K)	200	k_{s1} (W/m-K)	0.6
h_{∞} (W/m ² -K)	0.54	k_{s2} (W/m-K ²)	0
q_w (kW/m ³)	12	H^* (MJ/kg-K) [ASH]	0
T_{∞} (C)	25	H^* (MJ/kg-K) [WATER]	-15.88
l_w (cm)	3.81	H^* (MJ/kg-K) [ORG]	-4.6
q_w (kg/m ³)	8000	H^* (MJ/kg-K) [GORG]	0
c_w (J/kg-K)	480	c_{s1} (J/kg-K) [ASH]	1000
Sc	0.7	c_{s2} (J/kg-K ²) [ASH]	0
Pr	0.88	c_{s3} (J/kg-K ³) [ASH]	0
d_p (cm)	1	c_{s1} (J/kg-K) [WATER]	954
ϕ_e	0.5	c_{s2} (J/kg-K ²) [WATER]	-29
ϵ	0.8	c_{s3} (J/kg-K ³) [WATER]	0.0386
c_{g0} (J/mol-K)	30.36	c_{s1} (J/kg-K) [ORG]	1000
c_{g1} (J/mol-K ²)	9.615x10 ⁻³	c_{s2} (J/kg-K ²) [ORG]	0
c_{g2} (J/mol-K ³)	1.184x10 ⁻⁶	c_{s3} (J/kg-K ³) [ORG]	0
μ_0 (Pa-s)	-2.33x10 ⁻⁶	c_{s1} (J/kg-K) [GORG]	1000
μ_1 (Pa-s/K)	3.84x10 ⁻⁸	c_{s2} (J/kg-K ²) [GORG]	0
H (kJ/mol) [N ₂]	0	c_{s3} (J/kg-K ³) [GORG]	0
H (kJ/mol) [H ₂ O]	-241	ρ_{1s} (kg/m ³) [ASH]	1000
H (kJ/mol) [CO ₂]	-392.2	ρ_{2s} (kg/m ³) [WATER]	880
γ_l	1.0	ρ_{3s} (kg/m ³) [ORG]	1000
γ_h	0.0	ρ_{4s} (kg/m ³) [GORG]	1000
α_l	0.6	β	10
α_h	0.01	σ	1
A (1/s)	6.3x10 ⁴		
T_a (K)	10000		

The external heat transfer coefficient was chosen to simulate the approximately 10 cm of insulation on the outside of the vessel. The energy input to the wall provided by electrical heaters was only applied for the first 6.0x10⁴ s (16.7 hr). The average gas

property parameters were chosen to be those of water vapor, the dominant gas in the system during most of operational time.

The decomposition rate parameters are the same ones used in previous work¹. They were chosen to yield a time constant for decomposition of 10 minutes at 300 C and have a relatively low activation temperature. This means for an isothermal case about 50 minutes would be required to react 90% of the newspaper at 275 C. These reaction parameters are based on educated guesses at this point and limited experimental work. In reality, the decomposition reactions are much more complicated than the simple reaction modeled here. If it is necessary to model the reaction more completely, additional rate expressions can be added in a straightforward manner.

In the simulation three gas species were used: nitrogen to simulate the initial air in the system, carbon dioxide to simulate the primary noncondensable gas formed from the decomposition reaction, and water vapor the dominant gas. The heat of formation of the solid product of decomposition, GORG, was adjusted so that the heat of reaction for decomposition was 0.4 MJ/kg-ORG at 550 K, 0.23 MJ/kg-ORG at 298 K.. This is similar to values used in previous work¹. The effective heat of vaporization for water vapor, which the model calculates based on heats of formation and heat capacities, is within 2% of the actual value at low temperatures and 6% at 550 K.

Based on preliminary runs it was found that a computational grid 8x9, 8 cells in the radial direction, was a reasonable compromise between accuracy and run time. The computational cell sizes used, Table 2, are non uniform so that more resolution is available near the boundaries where interaction with the vessel wall is important. With this mesh, the model calculations took about 5.4 hours on an HP-9000/730 work station to compute the solution for 11+ day experiment. The computations were performed with an LSODE error tolerance parameter of 10^{-5} . This is the parameter which controls relative error during each time step of the solution. For typical problems this parameter is set between 10^{-4} and 10^{-6} . For this problem the solution ran into difficulty when the less restrictive 10^{-4} was tried.

Table 2. Cell sizes.

Radial Cell	Size (cm)	Vertical Cell	Size (cm)
		9	20
1	20	8	20
2	15	7	20
3	11	6	20
4	9.0	5	15
5	2.0	4	2.0
6	1.5	3	1.5
7	1.0	2	1.0
8	0.5	1	0.5

Computed average temperatures and pressures during the first phase of operation, the wall heating phase, are shown in Fig. 1. This phase lasts overnight, 16 hours, during which a relatively low wall heating rate of 2.3 kW provided by the electrical wall heaters. This brings the average vessel wall temperature to just under 150 C. Because of heat transfer from the wall to vessel contents, wet paper at the wall dries and heat is carried into the vessel. This raises the average temperature of the vessel contents to about 75 C and increases the pressure to just under 1.8 atmospheres. During this period no gas is allowed to leave the vessel.

Following the wall heating period active steam injection begins. As the steam heats the contents of the vessel the pressure in the vessel increases until it reaches the relief pressure. For this vessel that pressure is 6.3 MPa. At this point gas is produced from the vessel to maintain the pressure at 6.3 MPa. For the last part of the cycle the steam injection is reduced to a low level sufficient to help sweep gaseous products, formed by the decomposition reactions, out of the vessel. After a short period, the decomposition has been completed and the pressure is relieved. Computed pressures, temperatures, flow rate and vessel contents are plotted as function of time in Figs 2-4. Notice in Fig. 4 that the wall temperature lags behind the vessel contents temperature because of the large heat capacity of the steel walls and the reduced heat transfer which occurs as the wall region saturates.

Figure 1. Average wall temperature, vessel contents temperature and vessel pressure during the wall heating phase.

Figure 2. Steam injection and computed gas production rate during the active steam heating and pressure letdown phases.

Figure 3. Computed average wall temperature, vessel contents temperature and vessel pressure during the active steam heating and pressure letdown phases.

Figure 4. Computed average density of solids and water in the reactor vessel during the active steam heating and pressure letdown phases.

The results of these calculations compare fairly well with those estimated previously with the less complicated model¹ which treats the vessel in a lumped fashion. Selected results from the two models are compared in Table 3. The current model is referred to in the table as GSFS and the previous model as STM.

Table 3. A comparison of computed results from the 3D model, GSFS, and the simpler model, STM.

	GSFS Model Results	STM Model Results
Vessel water at end of steam injection (kg)	298	333
Vessel water after pressure letdown to 1 atmosphere (kg)	173	218

The GSFS model computes many things which are not addressed by the simpler model. This includes the spatial distribution of water during the operation. In Fig. 5, the computed water distribution as a function of distance from the wall is plotted for a position located approximately halfway up the side of the vessel. At the end of the wall heatup phase the model indicates that a layer of dried solid will extend into the originally wet newspaper 1 to 2 cm. At the end of the steam injection (labeled "end of heatup" in the plot) the computed water saturation has increased throughout the vessel and the layer near the wall extending out about 2 cm now has an elevated water content. This is caused by the extra steam condensation needed to heat the vessel walls from the 150 C to the maximum temperature of approximately 280 C. After the pressure is released and the system returns to 100 C, a dry layer again develops near the wall because of the heat available in the vessel walls which dries the near wall region. During the slow cooling process which follows, the wall region resaturates as heat is lost to the surroundings. A dry layer, however, is still present several centimeters away from the wall.

Figure 5. Computed water content near the vessel walls at the end of each major phase of operation.

The computed overall conditions in the vessel are plotted in Fig. 6 versus time for the extended cool off period. During this period the pressure in the vessel is below atmospheric pressure and heat is slowly lost from the vessel walls through the insulation to the surroundings. Because of the insulation, the cooling is slow and 10 days are required for the temperature of the vessel contents to drop to 40 C.

Calculations indicate that the rate of cooling can be increased considerably if a small bleed flow is begun after the pressure reaches one atmosphere. Computations done with a bleed flow of only 10 mmol/s of nitrogen show the temperature dropping to 40 C in a little over 4 days, see Fig 6. The additional cooling occurs is a result of the evaporation of water into the nitrogen steam. The nitrogen injection maintains the system pressure and allows the water vapor to be carried out of the vessel.

Figure 6. Computed cooling with and without a nitrogen sweep of 10 mmol/s.

The bed conductivity which is particularly important for the development of the wall region is computed according to correlations previously given. In this case computed conductivities range from a low of about 0.07 W/m/K to a high of about 0.8. Typical values for conditions in which the material has dried are about 0.15 W/m/K. The higher effective conductivity values are present when significant gas flows are present. For comparison the conductivity of saturated steam is 0.025 W/m/K at 100 C and 0.058 W/m/K at 280 C.

As part of the calculations internal gas velocities are computed within the vessel. It is important for actual operation of the pilot reactor that these velocities not be too large. Large velocities would lead to excessive pressure drop in the system and/or to entrainment of solid and liquid in gas exiting the vessel. Two measures of the computed gas velocities are shown in Fig. 7. One is the volume weighed average velocity and the other is the maximum velocity existing at any horizontal plane in the vessel. The highest velocities occur during the lowest pressure periods. The computed velocities are quite low, reaching only 0.04 m/s briefly during the pressure letdown phase. This spike could be reduced, if necessary, by a change in the valve opening schedule during the pressure letdown. These velocities should cause no significant pressure drops in the vessel and should result in little entrainment of solids.

To reduce the computational difficulties the algorithm for artificially changing the average bed permeability was employed. In this case the algorithm was employed which held the pressure drop to system pressure ratio within a set range. The bed permeability was initially set at $2 \times 10^{-12} \text{ m}^2$. This permeability was altered by the model according to the following:

$$\frac{\Delta P}{P} < 0.02 \text{ then } \Gamma_{new} = 0.5\Gamma,$$

$$\frac{\Delta P}{P} > 0.04 \text{ then } \Gamma_{new} = 1.5\Gamma.$$

The adjustments were only done when the inlet or exit flow was greater than 0.01 mol/s. This limit was imposed so that changes did not occur during periods of very low system flow. The adjustments were not done continuously but only after set time intervals. The time intervals varied depending on the experimental time but were between 100 and 200 seconds during the most active periods of the process. The resulting permeability changes during the active steam heating and pressure letdown phases are shown in Fig. 8. The permeability used ranged from a high of $23 \times 10^{-12} \text{ m}^2$ to a low of $0.04 \times 10^{-12} \text{ m}^2$, nearly a 3 orders of magnitude change.

As long as the pressure drop within the system is a small fraction of the system pressure the computed results should not be unduly influenced by the artificial changes in permeability. In Fig. 9 the ratio of overall pressure drop to average system pressure is plotted. It is seen that the permeability changing algorithm has kept the ratio small except during short periods at the beginning and end of the steam heating period. The spikes occur just as steam injection starts and just as production flow ends. Both these periods are low pressure operations and have a relatively short duration.

Because of the changes in permeability, the computed pressure drops in the bed are artificial. However, as part of the solution the product of overall pressure drop to existing permeability is computed. This result is shown as a function of time in Fig. 10. This product can be used to estimate what the pressure drop would be for a given constant bed permeability, or alternatively how permeable the bed would need to be to have a pressure drop less than a prescribed amount. In this case, a pressure drop of 10 kPa would be sufficient to lift the bed. Since the maximum pressure drop permeability product is $230 \times 10^{-9} \text{ kg-m/s}$, the minimum permeability to insure a pressure drop of less than 10 kPa would be $23 \times 10^{-12} \text{ m}^2$ (23.3 darcies). A bed composed of particles with a diameter of only 84 μm has a permeability of 23 darcies. Although the permeability of the shredded newspaper feed is not known, it is probably many thousands of darcies. Consequently, the calculations indicate that the pressure drop within the vessel under these conditions will be very small.

Figure 7. Computed velocities and system pressures during the active steam heating and pressure letdown phases.

Figure 8. Computed variation in permeability and average system pressures during the active steam heating and pressure letdown phases. Note, $0.987 \times 10^{-12} \text{ m}^2$ is one darcy.

Figure 9. Computed variation in the ratio of pressure drop (bottom to top of bed) and average pressure. during the active steam heating and pressure letdown phases.

Figure 10. Computed variation of the product of pressure drop and bed permeability. Note, $100 \times 10^9 \text{ kg-m/s}^2$ is about 100 kPa-darcy.

The primary driver for the changes occurring in the bed is the evaporation and condensation of water and steam. As outlined above, this essentially equilibrium driven process is approximated in the model using evaporation and condensation rates. In this case a σ rate parameter of one was used. This led to typical rates during condensation and evaporation as high as about 20 mol/s/m^3 . One measure of whether this rate is fast enough to simulate the equilibrium nature of the process is provided by looking at the difference between the system temperature and the equilibrium temperature at positions in the system where active condensation or evaporation is occurring. In most of the system the difference in these two temperatures was less than 1 C. At locations of high rates, at steam fronts and near the walls, this difference is as high as 6-10 C. These relative small departures from equilibrium should not unduly influence the computed results and therefore the rates used appear to be adequate.

It is possible to run the problem faster, i.e. less computer time, if the permeability in the very narrow zones near the wall are reduced by a factor of five. Since very narrow

zones are used near the wall, about 1 cm, to resolve the narrow drying zone the pressure differences between nodes near the wall are extremely small. Because the small pressure difference is what drives the flow away and to these zones problems can arise due to the inherent accuracy of the numerical solution. The reduction in permeability increases the pressure gradient near the wall and allows more accurate computation of gas fluxes. In many cases this artificially high permeability does not significantly degrade the accuracy of the overall solution (see Appendix I) with respect to overall performance of the system. In this case only 2.5 hr. were required for this same problem with reduced permeabilities near the wall rather than the 5.4 hr. of the unaltered case.

Commercial Scale System

In work reported in reference 2, it was shown that the overall performance of a direct-steam heat operation is degraded if it is assumed that the vessel contents are thermally coupled to the thick vessel walls. In that work it was argued that the development of a dry layer near the vessel walls could result in operations which may be more adiabatic, from the standpoint of the vessel contents, in nature and thus more favorable. The GSFS model has been used to take a preliminary look at the degree of coupling between the commercial scale vessel contents and their thick, 16 cm, metal walls.

The system modeled is equivalent to the operation shown schematically in Fig 11. This is the system in which two preheat beds are used to capture waste heat from gas exiting higher pressure vessels. This conceptual direct-steam heat process includes the following steps. The shredded and classified raw MSW is loaded into a pressure vessel. The vessel is sealed and steam is introduced to heat and pressurize the vessel. After maintaining the system at reaction temperature for the desired length of time the pressure is gradually reduced, turning part of the water to steam which cools the vessel contents. Gas exiting a reactor stage is used to preheat a companion vessel in an earlier stage of the sequence. After reaching atmospheric pressure, the reactor is unloaded.

The various stages of operation of the reactor vessel are labeled stage 1-6. Stage 1 (not labeled in the figure) is the atmospheric loading of the classified MSW into the vessel. Stage 2 is the steam heating of the MSW feed with gas produced during the intermediate pressure letdown, stage 5. Stage 3 is the second preheat stage in which gas produced from stage 4 is used to further heat the feed. Stage 4 is the final heating stage where high pressure steam is introduced to bring the system to the final desired temperature. Stage 6 is the final pressure letdown/cooling phase. The gas and steam from stages 2, 3 and 6 operations are sent to a condenser.

Included in Fig. 8 is the results computed using the ASPEN PLUS continuous simulator. In these results it was assumed that vessel contents did not transfer heat to the vessel walls.

Figure 11. ASPEN PLUS computed results for adiabatic 2 preheat bed conceptual commercial scale process.

The GSFS model was used to simulate the operation of vessel stages 2-6. In the calculations the vessel was assumed to be 4 meters in diameter and 8 meters high. This is a volume of 100 m³. It was assumed that the total density of the raw MSW feed was 500 kg/m³, and therefore the vessels could hold 50 Mg of raw feed. A residence time for each stage of 2000 s (33.3 min.) was used. This would give a total throughput of 25 kg/s of raw MSW. Most other parameters, see Table 4, are the same as those used in the pilot simulation with only a few exceptions. The primary difference is in the wall parameters. The vessels are thicker and no active heating is used. The initial wall temperature is high because the vessels move through a sequence of operations and walls do not fully cool (see results below) before a new sequence begins.

Table 4. Model parameters used in full scale calculations, those marked with an "•" are different than the values used in the pilot simulation.

Parameter	Value	Parameter	Value
h_w (W/m ² -K)	200	k_{s1} (W/m-K)	0.6
h_{∞} (W/m ² -K) •	0	k_{s2} (W/m-K ²)	0
q_w (kW/m ³) •	0	H^* (MJ/kg-K) [ASH]	0
T_{∞} (C) •	201	H^* (MJ/kg-K) [WATER]	-15.88
l_w (cm) •	15	H^* (MJ/kg-K) [ORG]	-4.6
q_w (kg/m ³)	8000	H^* (MJ/kg-K) [GORG]	0
C_w (J/kg-K)	480	C_{s1} (J/kg-K) [ASH]	1000
Sc	0.7	C_{s2} (J/kg-K ²) [ASH]	0
Pr	0.88	C_{s3} (J/kg-K ³) [ASH]	0
d_p (cm)	1	C_{s1} (J/kg-K) [WATER]	954
ϕ_e •	0.3	C_{s2} (J/kg-K ²) [WATER]	-29
ϵ	0.8	C_{s3} (J/kg-K ³) [WATER]	0.0386
C_{s0} (J/mol-K)	30.36	C_{s1} (J/kg-K) [ORG]	1000
C_{s1} (J/mol-K ²)	9.615x10 ⁻³	C_{s2} (J/kg-K ²) [ORG]	0
C_{s2} (J/mol-K ³)	1.184x10 ⁻⁶	C_{s3} (J/kg-K ³) [ORG]	0
μ_0 (Pa-s)	-2.33x10 ⁻⁶	C_{s1} (J/kg-K) [GORG]	1000
μ_1 (Pa-s/K)	3.84x10 ⁻⁸	C_{s2} (J/kg-K ²) [GORG]	0
H (kJ/mol) [N ₂]	0	C_{s3} (J/kg-K ³) [GORG]	0
H (kJ/mol) [H ₂ O]	-241	ρ_{1s} (kg/m ³) [ASH]	1000
H (kJ/mol) [CO ₂]	-392.2	ρ_{2s} (kg/m ³) [WATER]	880
γ_l	1.0	ρ_{3s} (kg/m ³) [ORG]	1000
γ_h	0.0	ρ_{4s} (kg/m ³) [GORG]	1000
α_l	0.6	β	10
α_h	0.01	σ	1
A (1/s)	6.3x10 ⁴		
T_a (K)	10000		

A grid system consisting of 9 cells in the vertical direction, with equal spacing between nodes, and 8 cells, with variable node spacing (see Table 5), in the radial direction was used in simulating the problem. A number of narrow zones were used near the wall to resolve wall interactions. The run time was 2.3 hours using an LSODE tolerance of 10^{-5} . Because of the large size of the system, the thin wall zones led to computational problems when the permeability of the system was uniform. To overcome this problem the thin wall zones, 6-8, were given a permeability which was maintained at 20% of the remainder of the system. This allowed the computations to be successfully completed.

Table 5. Cell sizes for full scale simulations.

Radial Cell	Size (cm)	Vertical Cell	Size (cm)
1	70	1	50
2	71	2	100
3	35	3	100
4	29	4	100
5	8	5	100
6	4	6	100
7	2	7	100
8	1	8	100
		9	50

Computed flow rates, average temperatures and pressures are shown for all 5 stages in Figs. 12-15. Note that the flow from stage 5 feeds stage 2 and from stage 4 feeds stage 3. Since the computations moves forward in time an iterative process is needed to define the inputs to stages 2 & 3. This iteration was only approximate in the results shown. That is, the input to stages 2 & 3 are consistent with the computed output of stages 4 & 5, but not exactly equivalent. The wide variation in flow rates is primarily a result of the pressure schedule used during pressure letdown operations. This schedule was tailored to minimize velocities within the vessel.

Figure 12. Computed results for all five stages of a 2 preheat bed system (end times of stages in minutes: 2-33.3, 3-66.6, 4-99.9, 5-133.2, & 6-166.5).

Figure 13. Computed results for all five stages of a 2 preheat bed system. The label "Average Temperature" refers to the vessel contents.

Figure 14. Computed results for all five stages of a 2 preheat bed system. The raw MSW organic mater is labeled ORG and the product of the hydrothermal decomposition of this organic mater is labeled GORG.

The computed results indicate that the coupling between vessel contents and vessel walls is not great. The computations indicate that the average wall temperature would stay close to 200 C, see Fig. 13. The weak coupling is a result of the short residence times in each stage and the development of dried zones right at the vessel walls during certain phases of the operation. This dry zone has a low thermal conductivity, estimated by the model to be on the order of 0.2 W/m/K.

The computed behavior of the system with respect to water saturation in the vicinity of the walls is shown in Fig. 15 at the end of operation of each stage. Notice that at the end of stages 2, 3 & 6 a narrow dry layer near the wall develops. This dry layer limits the heat transfer from the walls to contents of the vessels and effectively insulates the walls. Remember, this result is obtained using a model in which the water is assumed to be immobile. If water is actually mobile and moves into the dry layer then the coupling would increase.

Figure 15. Computed water content near the vessel walls at the end of each stage of operation.

Previously (reference 2) estimates were made of velocities within the vessels, and it was concluded that operation of stage 6 would lead to the highest internal velocities. In the GSFS calculations it is seen that stage 2 could also exhibit high velocities. As mentioned above some tailoring of the pressure letdown schedule was done to minimize internal velocities. Fig. 16 indicates that the pressure letdown schedule for stage 6 leads to a more or less constant velocity. Since a given amount of cooling, and thus steam flow, is required in stage 6 a process with a constant velocity minimizes the maximum velocity present. The spiky nature of the velocity during stage 6 is a result of the exact pressure letdown scheme. With more work a scheme could be devised which led to a smoother operation. Consequently, it is probably most appropriate to look at the average behavior which means maximum velocities of about 0.15 m/s develop during the stage 6 letdown.

The potential for entrainment of liquid droplets or solid particles is a function of the kinetic energy of the flowing gas. In Fig. 17 the product of gas density and superficial velocity squared is plotted as a function of time. This plot indicates that the beginning of stage 6 is the time when entrainment of liquids and solids is most likely. At time=140, the gas in the bed has an average superficial velocity of 0.15 m/s and the pressure and temperature of the system are 180 C and 0.96 MPa respectively. Under these conditions droplets on the order of 60 μm could be entrained. Whether such droplets or particles would be formed and then entrained is not known. Particle formation and entrainment would be specific to the details of the operation which are unknown at this time.

Figure 16. Computed velocities within the reactor vessel.

Figure 17. Computed average pressure and computed variation of the product of gas density and the square of the maximum average superficial velocity at a horizontal plane.

As in the pilot simulation, an algorithm was employed to artificially modify the bed permeability to maintain sufficient pressure drop so as to not cause undue computational difficulties. The same basic algorithm was used as was described above for the pilot simulation except that since the system is so much larger a minimum flow of 1 mol/s was used, below which no changes were made. Also, the permeability was

limited to a maximum value of $200 \times 10^{-12} \text{ m}^2$. In Figures 18 and 19 the permeability and pressure drop/pressure ratio are plotted. The permeability initially was set at $200 \times 10^{-12} \text{ m}^2$. The lowest value reached was about $0.7 \times 10^{-12} \text{ m}^2$. The algorithm did a good job in maintaining the ratio of pressure drop to pressure near the desired 0.02 level. The exceptions are during the low pressure operation at the beginning and end of the experiment. However, it was not a failure of the algorithm, but the constraint of a maximum permeability which accounted for the large ratios. The simulation assumes that the bed actually has a permeability of $200 \times 10^{-12} \text{ m}^2$ and consequently the pressure drops computed at the end and the start are real, and the model appropriately accounts for them.

Figure 18. Gas injection rates, computed gas production rates and variation of permeability. Note, $0.987 \times 10^{-12} \text{ m}^2$ is one darcy.

Figure 19. Computed average pressure and computed variation of the ratio of pressure drop to average pressure.

The computed permeability pressure drop product is shown in Fig. 20. In this case the vessels are large and a pressure drop of 50-100 kPa would be needed to lift the bed. Assuming 100 kPa is the upper limit of pressure drop which can be tolerated the bed would need to have a permeability of greater than $180 \times 10^{-12} \text{ m}^2$ to maintain the pressure drop at acceptable levels. Beds of MSW would probably be at least this permeable initially, but as they saturated effective permeabilities in this range may be approached. Accordingly, it is not possible to discount completely bed permeability as a limiting factor in operation of large scale systems. Experimental data would have to be gathered to answer the question. Strategies to mitigate the constraint of pressure drop would include longer operational times and multiple gas injection and production locations within the vessels.

Figure 20. Gas injection rates, computed gas production rates and computed variation of the product of pressure drop and bed permeability. Note, $100 \times 10^9 \text{ kg-m/s}^2$ is about 100 kPa-darcy.

A Single Vessel

Calculations have also been performed for a commercial scale system in which heat recovery is not part of the process. This is conceptually a simpler operation in that the MSW is loaded into a reactor vessel and then heated with high pressure steam. The pressure letdown phase is shorter because there is less constraint on acceptable flow rates than is present when heat recovery is used.

All parameters used in the calculations were the same as those used in the 2 preheat bed case except for scheduling of flows and pressures. The model required approximately 100 minutes of computer time to complete the 140 minute simulation. Absent the narrow wall cells the calculations require one-tenth the time. It is shown in Appendix II that results without wall zones yields many overall results consistent with the more time consuming result in which the wall zone is resolved.

Computed results are presented in Figs 21-27. In this case higher maximum flow rates of steam were used than in the 2 preheat bed case. This was done to reach reaction temperature as rapidly as possible. Once the desired temperature, 300 C in this case, was reached the steam injection was dropped to a level where it would be adequate to sweep out product gas and maintain the 300 C temperature. The low initial steam flow was used to limit internal velocities and pressure drops.

Figure 21. Steam injection and computed gas production rate for a 100 m^3 vessel.

Figure 22. Computed average wall temperature, system temperature and system pressure for a 100 m^3 vessel.

Figure 23. Computed vessel contents for a 100 m³ vessel.

Figure 24. Computed velocities within the reactor vessel for a 100 m³ vessel.

Figure 25. Computed pressure drop from inlet to exit plane and average system pressure for a 100 m³ vessel.

Figure 26. Steam injection rates, computed gas production rates and variation of permeability for a 100 m³ vessel.

Figure 27. Computed average pressure and computed variation of the ratio of pressure drop to average pressure for 100 m³ vessel.

Figure 28. Steam injection rates, computed gas production rates and computed variation of the product of pressure drop and bed permeability for 100 m³ vessel.

Although no iteration for flows is needed in this case the initial wall temperature was set based on the value it reached at the end of cycle. This was done assuming that a reactor would be in more or less continuous operation. Careful examination of Fig. 22

will show that the initial wall temperature is 185 C, while the final temperature is only 181 C. This closure was deemed adequate although another loop could have probably brought it to within one degree.

The length of the time the reactor is held at high pressure was adjusted to give a system in which nearly all the initial ORG (96%) has decomposed. The time at a temperature of 300 C or over is about 45 minutes.

The size of the internal velocities are similar to those for the 2 bed case. During the initial steam injection period the velocities are somewhat higher than the two bed case. These could be lowered by using a lower initial injection rate of steam, however this would lengthen the total required time for the entire heating, reacting and cooling sequence. The particular steam injection schedule used is not necessarily the optimum. An optimized steam schedule would require additional information including the true limitations of exact bed permeability, tolerable pressure drop levels, and acceptable internal velocities. Overall process economics would have to be considered to determine tradeoffs between total time, reactor costs, and a steam capacity.

As in the 2 preheat bed case the bed permeability was assumed to be $200 \times 10^{-12} \text{ m}^2$, and the permeability changing algorithm was setup with this as the upper limit. During the initial and final low pressure periods the permeability is at this limit so the computed pressure drops, Fig. 25, would be the actual pressure drops in a $200 \times 10^{-12} \text{ m}^2$ bed (about 200 darcies).

Conclusions

A general purpose packed bed model initially developed for coal gasification systems has been modified to allow calculations relating to the hydrothermal treatment of MSW to be performed. The model can compute spatially resolved gas flows, thermal evolution and decomposition reactions within a hydrothermal reactor. Through the use of artificial permeability changes the model is able to follow the evolving system through pressure changes of nearly two orders of magnitude. In some cases spatial variations in this artificial permeability were required to allow successful simulation of large scale systems with reasonable expenditures of computer time.

The model was applied to commercial and pilot scale systems. The pilot scale system, about 1 m^3 , in volume was simulated for a time span of approximately 11 days. This computation required approximately 5.4 hr. of computer time on a HP-9000/730 work station. Among other things the simulation indicated that velocities within the reactor pilot reactor vessel would be low for the operational scenario simulated. Also, the pressure drops within the vessel should be small as long as the bed permeability remains at $23 \times 10^{-12} \text{ m}^2$ (about 23 darcy) or higher. In addition, simulations with and without the use of a small nitrogen bleed introduced to the vessel after the vessel pressure drops to 1 atmosphere indicate that the cooling time can be reduced from 10 days to about 4 days if a small nitrogen bleed is introduced

The commercial scale system simulated had a hydrothermal reactor vessel size of 100 m³. Simulations of a systems representing a single bed system and multiple bed heat recovery systems were performed. The multiple bed simulations required 2.3 hours of computer time to simulate the entire sequence of operations spanning 10⁴ seconds, about 170 minutes. The single bed system required 100 minutes of computer time to simulate the 140 minute operational time.

The commercial scale results indicate that in the absence of flow of liquid water the coupling between the vessel contents and the thick metal walls should be relatively small and thus will not degrade the system performance. On the other hand the computed gas velocities are considerably larger than for the smaller pilot scale system and could potentially cause unwanted entrainment of liquid and solids, or could require processing times to be extended.

It appears that the model is capable of addressing some of the more detailed questions related to direct-steam heating of MSW. The model has difficulties in certain cases because of the large changes in system pressures present in typical hydrothermal reactor simulations. These problems are partially overcome in the model by the use of artificial permeability modifications. Based on results to date it appears that the model will prove to be a useful tool in our continued process development activities.

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NOMENCLATURE

A	Arrhenius pre-exponential term in decomposition reaction
c_e	Molar concentration of water vapor at in equilibrium with water at a given temperature
$c_{g0}, c_{g1} \text{ \& } c_{g2}$	Coefficients in 2 nd order temperature polynomial for gas molar heat capacity
$c_{s1}, c_{s2} \text{ \& } c_{s3}$	Coefficients in 2 nd order temperature polynomial for solid heat capacity (one set for each solid)
c_w	Heat capacity of vessel walls
c_i	Molar concentration of gas species i in the gas filled space
C	Molar gas concentration in gas filled space
d_p	Effective particle size
D	Effective mass dispersion in the bed
D_a	Effective mass dispersion in the direction of gas flow
D_g	Average gas diffusivity
D_p	Effective mass dispersion in the direction perpendicular to gas flow
f_i	Prescribed injection gas flux of species i
G	Gas outflow flux
h_i	Molar enthalpy of gas species i
h_k^*	Enthalpy, per unit mass, of solid species k
h_w	Heat transfer coefficient from vessel contents to wall
h_∞	Heat transfer coefficient from vessel walls to surroundings
H	Molar heat of formation of gas species (one for each gas)
H^*	Heat of formation, per unit mass, of solid species (one for each solid)
j_i	Molar flux of gas species i
k	Effective thermal conductivity of bed
k_a	Effective thermal conductivity of bed in the direction of gas flow
k_0	Effective thermal conductivity of bed with no gas flow
k_g	Average gas thermal conductivity
k_r	Rate constant for decomposition reaction
k_p	Effective thermal conductivity of bed in the direction perpendicular to gas flow
k_s	Modified particle thermal conductivity
$k_{s1} \text{ \& } k_{s2}$	Coefficients in the 1 st order temperature polynomial for solid thermal conductivity
l_w	Thickness of vessel walls
P	Pressure

P_o	Pressure of gas outlet sink
Pr	Average gas Prandtl number
q_w	Heat input to vessel walls per unit volume
Q_i	Rate of introduction of gas species i into the bed
U	Superficial gas velocity
v	Effective gas velocity
v_{int}	Interstitial gas velocity
V_p	Number of particles per unit volume of bed
s_i	Source rate of gas i from reactions
s_k^*	Source rate of solid k from reactions
Re	Reynolds number based on superficial velocity and particle diameter
Sc	Average gas Schmidt number
t	Time
T	Temperature
T_a	Arrhenius activation temperature in decomposition reaction
T_w	Wall temperature
T_∞	Temperature of surroundings
y_i	Mole fraction of gas species i
W	Heat source strength per unit bed volume
α	Pseudosaturation
α_i & α_h	Pseudosaturation parameters used in bed relative permeability relation
β	Gas outflow parameter
γ_i & γ_h	Parameters used in bed relative permeability relation
Γ	Bed permeability
ε	Solid emissivity
η	Direction perpendicular to the wall
μ	Gas viscosity
μ_0 & μ_1	Coefficients in the 1 st order temperature polynomial for gas viscosity
ρ_g	Average gas density
ρ_k	Density of solid k per unit volume of bed
ρ_{k_s}	Intrinsic density of solid species k
σ	Scale factor for water condensation rate
ϕ	Void fraction
ϕ_e	Void fraction external to particles
ϕ_e^o	Initial void fraction external to particles
ϕ_{int}	Gas filled porosity internal to particles

APPENDIX I

COMPARISON OF UNIFORM PERMEABILITY AND LOW WALL ZONE PERMEABILITY CALCULATIONS

In many cases fine zones are needed near the wall to resolve interactions between the bulk material and the wall. Consequently the pressure differences between nodes near the wall can become extremely small. Because the small pressure difference is what drives the flow away from and to these zones problems can arise due to the inherent accuracy of the numerical solution. To reduce the computational difficulty and/or save computational time the permeability of the narrow zones at the wall can be increased. The reduction in permeability increases the pressure gradient near the wall and allows more accurate computation of gas fluxes. In many cases this artificially high permeability does not significantly degrade the usefulness of the overall solution.

Computations have been carried out for a pilot scale system. The system of interest is a cylindrical reactor vessel 1.3 m in diameter and 1 m high. The cell sizes used in the simulation are given in Table I-1. The cells near the walls are much narrower than those in the interior. In one case all cells were given the same permeability at any instant in time, while in the other case the permeability of radial cells 5-8 and vertical cells 1-4 were given a permeability 20% of that of the interior.

Table I-1. Cell sizes.

Radial Cell	Size (cm)	Vertical Cell	Size (cm)
		9	20
1	20	8	20
2	15	7	20
3	11	6	20
4	9.0	5	15
5	2.0	4	2.0
6	1.5	3	1.5
7	1.0	2	1.0
8	0.5	1	0.5

In Figure I-1 to I-11 overall results of the simulations are plotted for both the uniform case and the low wall permeability case. For the most part these plots indicate that the two solutions give similar results. The average pressure, average temperature, average velocities and amount of ORG as a function of time show essentially no differences for the two cases. The most significant differences occur in the product gas flow rate, the average wall temperature and the water content. The largest percentage difference in the water content is about 3.5% at the 18.5 hour mark. Some of the other percentage differences are larger, but these are generally for parameters during rapid transients. The pressure drop, Fig I-10, shows a consistent difference during the period of high

pressure operation. This difference is small, 20 kPa, compared to the operating pressure of 6 MPa. The increase in pressure drop is consistent with change in effective area for vertical gas flow. The increase in pressure drop is about 13% while the area of decreased permeability near the wall is about 16%.

Figure I-12 shows that the increase in computational time occurs, as one would expect, during the active periods of the process. Relatively little computational time is needed to cover the prolonged cool down period. The constant permeability case requires just over twice as much total computational time.

In Figures I-14 to I-16 the water content of the zone near the wall are compared for the two cases. Since the wall zone is the area in which the permeability has been artificially lowered one might expect that any changes would be reflected in differences in the water profile near the wall. These results show some differences but none of real significance. The largest difference shows up at the 19.9 hours mark, just at the end of the active steam injection period.

It appears that the use of a lower permeability zone near the wall to reduce computational difficulty probably does not lead to unacceptable differences in computed results in this case. This suggests that it can be used in other cases to obtain reasonable results when computations fail for the constant permeability case.

Figure I-1. Computed average system pressure during the active steam heating period.

Figure I-2. Computed exit gas flow rate during the active steam heating period.

Figure I-3. Computed average temperature of the vessel contents during the active steam heating period.

Figure I-4. Computed average wall temperature during the active steam heating period.

Figure I-5. Computed mole fraction of carbon dioxide in the exiting gas during the active steam heating period.

Figure I-6. Computed average water content during the active steam heating period.

Figure I-7. Computed average ORG content during the active steam heating period.

Figure I-8. Computed average velocity inside the vessel during the active steam heating period.

Figure I-9. Computed average velocity across a horizontal plane during the active steam heating period.

Figure I-10. Computed pressure drop from inlet to outlet plane during the active steam heating period.

Figure I-11. Interior bed permeability during the active steam heating period.

Figure I-12. Computer run time as a function of experimental time.

Figure I-13. Computed water content near the vessel wall at the end of the initial wall heating period.

Figure I-14. Computed water content near the vessel wall at the end of the active steam injection period.

Figure I-15. Computed water content near the vessel wall at the end of the initial cooling period.

Figure I-16. Computed water content near the vessel wall at the end of the run.

APPENDIX II

COMPARISON OF ZERO PREHEAT BED RESULTS

Several runs were done for the commercial scale hydrothermal reactor vessel, 4 m diameter and 8 m high, to explore the importance of error tolerance selection and to indicate the influence of small grid spacing near the wall on the computed results.

The base case calculations were done using the grid shown in Table II-1 and a LSODE tolerance parameter of 10^{-4} . One model run was done in which the LSODE error tolerance was set at 10^{-5} . This base case took about 100 minutes of computer time. Interestingly the same problem musing an error tolerance of 10^{-4} case took a similar time. Results for basic process parameters as a function of time were similar. The following summarizes the differences in results for the two cases, periods of extreme change were exempted:

- Total water in the system differed by 1.5% or less, the maximum difference occurred near the end of the stem injection period
- The carbon dioxide content of the produced gas differed by 2% or less
- The average wall temperature differed by about 2%
- The average gas velocity and the average gas velocity at a horizontal plane differed by less than 1% except during on brief time period when they differed by about 5%.
- The following differed by less than 1%
 - Average system pressure
 - Average system temperature
 - Amount of ORG
 - Amount of GORG

Table II-1. Cell sizes for fine wall grid case.

Radial Cell	Size (cm)	Vertical Cell	Size (cm)
1	70	1	50
2	71	2	100
3	35	3	100
4	29	4	100
5	8	5	100
6	4	6	100
7	2	7	100
8	1	8	100
		9	50

This result indicates that if a given problem will run with the 10^{-4} tolerance the overall results are probably sufficiently accurate. The primary motivation for using the less restrictive tolerance would be the savings in run time. Since the savings in this case is zero the first tolerance tried for a problem should probably be 10^{-5} .

The same problem was run with a coarse grid in the radial direction, Table II-2. Based on model parameters it is clear that this grid cannot resolve the wall layer. However, larger and fewer nodes, especially in the radial direction, can greatly increase the speed of calculations. For this case the coarse grid took only 10 minutes of computer time, compared to 100 minutes for the finer zone. The increase in computation speed is larger than the decrease in computational cells because the presence of thin cells near the wall require more computational effort than the average bulk cell.

Table II-2. Cell sizes for coarse grid case.

Radial Cell	Size (cm)	Vertical Cell	Size (cm)
1	25	1	50
2	50	2	100
3	50	3	100
4	50	4	100
5	25	5	100
		6	100
		7	100
		8	100
		9	50

The injected steam flow for both cases is given in Fig. II-1. In Figures II-1 to II-11 the computed results for parameters as a function time are compared for the two cases. Certain overall aspects of the computed results, such as the system pressure, average temperature, and the amount of water and ORG are very similar for the two cases. Others vary by 10-20% and of coarse the water content at and near the wall are quite different, Table II-3.

Table II-3. Compute water content at the outer wall halfway up the vessel.

Time (min.)	Water at the Wall (kg/m ³)	
	Fine Wall Grid	Coarse Grid
0	125	125
20	0	163
40	355	361
60	471	449
80	475	315
133	0	184

Figure II-1. Steam injection flow rate.

Figure II-2. Computed average system pressure.

Figure II-3. Computed exit gas flow rate.

Figure II-4. Computed average temperature of the vessel contents.

Figure II-5. Computed average wall temperature.

Figure II-6. Computed mole fraction of carbon dioxide in the exiting gas.

Figure II-7. Computed average water content.

Figure II-8. Computed average ORG content.

Figure II-9. Computed average velocity inside the vessel.

Figure II-10. Computed maximum average velocity across a horizontal plane.

Figure II-11. Computed pressure drop from inlet to outlet plane.

Figure II-12. Interior bed permeability.

Figure II-13. Computer run time as a function of experimental time.

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