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Gasification of Sewage Sludge: Mathematical Modelling of an Updraft Gasifier

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In this paper, a one-dimensional unsteady state mathematical model for the simulation of a small scale fixed-bed updraft gasifier is presented. The model is based on a set of differential equations which couples heat and mass transport in the solid and gas phases with sewage sludge drying and devolatilization, char gasification and combustion of both char and gaseous species. The model was used to simulate the behavior of sewage sludge with 20 % moisture in an updraft fixed-bed gasifier (2 m height, 0.165 m i.d.) of a pilot-scale plant operating at atmospheric pressure. Good agreement was achieved between predictions and experimental measurements for the dynamic axial temperature profiles and the steady state composition of the producer gas.

1. Introduction

Two main classes of chemical reactors, fixed-bed and fluid-bed reactors, are applied for biomass gasification. Fixed-bed (updraft and downdraft) reactors are of very simple construction and operation. They present high carbon conversion, long solid residence times and low ash carry-over. The updraft reactors are more thermally efficient and present easy scalability than the downdraft process. Numerous models of these reactors have been proposed for the coal and biomass gasification, since this technology is applied for 89 % of the coal gasified in the world. Several industrial updraft gasifiers are in operation in Norhern Europe for wood chips gasification (Di Blasi, 2004). However, no experimental analysis is currently available in literature on updraft gasification of sewage sludge and the few models proposed for sewage sludge gasification are about pilot-scale circulating fluidized bed (Petersen and Werther, 2005). In this study, an unsteady mathematical model was presented that is comprehensive of the main physical and chemical processes of an updraft fixed-bed gasifier of sewage sludge, a potential fuel whose behaviour has not yet simulated in this type of reactor. Simulations were carried out for a pilot scale plant and a comparison between model predictions and measurements was provided.

2. Mathematical model

2.1 Governing equations

The gasification processes are modeled by means of one-dimensional (reactor axis) and unsteady differential mass and energy balances for the solid and gas phases. The model applies the conservative equations to a differential volume ΔV , which diameter equal to reactor diameter and height Δz , along the gasifier. Radial gradients are not considered as the residence time of the solids in the bed is long. Turbulence is not treated formally in the slowly moving bed with low gas velocities, but is included implicitly through the correlations for the effective heat/mass transfer coefficients. The momentum balance is not considered; thus, the gasifier is assumed to be isobaric. The particles fed are considered spherical and having the same average size, and the porosity of the bed is assumed constant along the gasifier.

The main processes modeled include: moisture evaporation by a 1st order kinetic equation; devolatilization of sewage sludge described by one step global reaction; finite-rate gas-phase water-gas shift; combustion of volatile species and tars; heterogeneous reactions of gasification (steam, carbon dioxide and hydrogen)

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and combustion of char; heat and mass transfer across the bed by convection and heat transfer between solid-gas, solid-wall and gas-wall. Because of the high ash content of sewage sludge (typically 30-40 % on dry basis), the heterogeneous reactions of the char have been modeled by means of the unreacted core model with constant shrinking particle size assuming that an ash layer remains intact on the particles. The gas species must diffuse through the external gas film boundary layer and then the ash layer before they react with the char. Assuming that no fragmentation, attrition or agglomerations of particles takes place, the bed porosity is constant and adopting the shell progressive model with constant particle size, the solid velocity results constant along the bed.

The raw sewage sludge is composed by volatiles, carbon fixed, moisture and ash. To be able to describe the drying, the devolatilization and the char combustion/gasification separately, the components of the solid were treated as independent components. So, four different solid species are considered: dry ash free sewage sludge (dafSS), moisture (M), char (C) and ash (A). Eleven gaseous components are considered to represent the gasification gas: oxygen (O_2) , nitrogen (N_2) , water (H_2O) , carbon dioxide (CO_2) , carbon monoxide (CO), hydrogen (H₂), methane (CH₄), ethane (C₂H₆), hydrogen sulphide (H₂S), ammonia (NH₃) and tar (T). Benzene was chosen as the model component of the tar because it was determined earlier as the major component in the producer gas representing 60-80 % of the total tar. The solid phase is characterized by the partial densities ρ_i (kg/m³_{bed volume}) for i = dafSS, M, C and A, solid velocity us (m/s) and temperature Ts (K). Similarly, the gas phase is characterized by the partial densities pi (kg/m³gas volume) for j = O₂, N₂, H₂O, CO₂, CO, H₂, CH₄, C₂H₆, H₂S, NH₃ and T, gas velocity u_g (m/s) and temperature T_{α} (K). The volatiles are assumed to behave as ideal gases. The basic equations are:

Mass conservation of solid-phase species

Daf SS
$$\frac{\partial \rho_{dafSS}}{\partial t} = -\frac{\partial (u_s \rho_{dafSS})}{\partial z} - R_{dev}$$
(1)

isture
$$\frac{\partial \rho_{\rm M}}{\partial t} = -\frac{\partial (u_{\rm s} \rho_{\rm M})}{\partial z} - R_{\rm dry}$$
 (2)

Char

Ash

$$\frac{\partial \rho_{\rm C}}{\partial t} = -\frac{\partial (u_{\rm s} \rho_{\rm C})}{\partial z} + \alpha_1 \cdot \frac{M_{\rm C}}{M_{\rm dafSS}} \cdot R_{\rm dev} - M_{\rm C} \sum_{i=1}^4 R_{\rm si}$$
(3)

$$\frac{\partial \rho_{\rm A}}{\partial t} = -\frac{\partial (u_{\rm s} \rho_{\rm A})}{\partial z} \tag{4}$$

Mass conservation of gas-phase species

$$\varepsilon \frac{\partial \rho j}{\partial t} = \frac{\partial (\varepsilon u_g \rho_j)}{\partial z} + M_j \sum_{k}^{N_R} v_{jk} R_k$$
(5-15)

Energy balances for the solid and gas phases

$$\sum_{i=1}^{4} \frac{\partial \rho_{i} H_{si}}{\partial t} = -\sum_{i=1}^{ns} \frac{\partial u_{s} \rho_{i} H_{si}}{\partial z} - Q_{sg} - Q_{sw} + (-\Delta H_{dry}) R_{dry} + \sum_{i=1}^{4} (-\Delta H_{Rsi}) R_{si}$$
(16)

$$H_{si} = cp_{si}(T_{s} - 298.15) \qquad i = dafSS, M, C, A$$

$$\sum_{j=1}^{11} \varepsilon \frac{\partial \rho_{j}H_{gj}}{\partial t} = \sum_{i=1}^{ns} \varepsilon \frac{\partial u_{g}\rho_{j}H_{gj}}{\partial z} + Q_{sg} - Q_{gw} + \sum_{l=1}^{N_{Rg}} (-\Delta H_{1})R_{1} \qquad (17)$$

$$H_{gj} = cp_{gj}(T_s - 298.15) \qquad j = O_2, N_2, H_2O, CO_2, CO, H_2, CH_4, C_2H_6, H_2S, NH_3, T$$

$$Q_{sg} = h_{sg}A_{sg}(T_s - T_g)$$
 $Q_{sw} = \frac{4h_{sw}}{D}(T_s - T_w)$ $Q_{gw} = \frac{4h_{gw}}{D}(T_g - T_w)$ $A_{sg} = \frac{6(1-\epsilon)}{d_p}$

Ideal gas law

$$\sum_{j=1}^{11} \frac{\rho_j}{M_j} = \frac{P}{R \cdot T_g}$$
(18)

Constant solid velocity us = usⁱⁿ

(19)

2.2 Kinetics

As in previous studies, the drying process was described by a 1st order kinetic equation depending on the temperature of the solid by means of an Arrhenius kind expression. The devolatilization of sewage sludge is a complex phenomenon, which involves a large number of chemical reactions. It is assumed that the total yield of char and volatiles equals the carbon fixed and volatile matter of the parent fuel, respectively, determined by the proximate analysis. The global pyrolysis rate is modeled as a first-order reaction with respect to the remaining volatile matter using the kinetic model proposed by Shao et al. (2008). In the model, pyrolysis was considered as an one step global reaction and is expressed as follows:

$$\begin{split} C_{\alpha}H_{\beta}O_{\gamma}N_{\delta}S_{\epsilon} \cdot A &\xrightarrow{\mu} \alpha_{1}CHAR \cdot A + [\xi_{H_{2}} \cdot \frac{\beta}{2}]H_{2} + [\xi_{CH_{4}}(\alpha - \alpha_{1})]CH_{4} + \xi_{CO}(\alpha - \alpha_{1})]CO + \\ [\gamma - (\xi_{CO} + 2\xi_{CO_{2}})(\alpha - \alpha_{1})]H_{2}O + [\xi_{CO_{2}}(\alpha - \alpha_{1})]CO_{2} + \epsilon H_{2}S + [(1 - \xi_{NH_{3}})\frac{\delta}{2}]N_{2} + \\ + [\frac{\beta}{4}(1 - \xi_{H_{2}}) + \frac{1}{4}(3\xi_{CO} + 5\xi_{CO_{2}} - 3\xi_{CH_{4}} - 1)(\alpha - \alpha_{1}) - \frac{1}{2}(\gamma + \epsilon) - 0.75\xi_{NH_{3}}\delta]C_{2}H_{6} + \xi_{NH_{3}}\delta NH_{3} + \\ [-\frac{\beta}{12}(1 - \xi_{H_{2}}) + \frac{1}{6}(\gamma + \epsilon) + \frac{1}{4}\xi_{NH_{3}}\delta + \frac{1}{12}(3 + \xi_{CH_{4}} - 5\xi_{CO} - 7\xi_{CO_{2}})(\alpha - \alpha_{1})]C_{6}H_{6} \end{split}$$

For computational simplicity, the composition of the volatile products is assumed to remain constant independently of the release rate and the char consists of pure carbon. α , β , γ , δ , ε are the mole fraction of component C, H, O, N, S in the dry ash free fuel (ultimate analysis). Five splitting factors are introduced to determine the stoichiometry of the pyrolysis reaction: ξNH_3 for the part of the nitrogen reacting to NH₃; ξCO for the part of the volatile carbon reacting to CO; ξ CO₂ for the part of the volatile carbon reacting to CO₂; ξ CH₄ for the part of the volatile carbon reacting to CH₄; ξ H₂ for the part of the hydrogen reacting to H₂. The composition of pyrolysis gas is strongly dependent on the sewage sludge variety, sample size and heating conditions. Therefore, the splitting factors were considered as open parameters and their values were obtained by fitting the model calculations to experimental producer gas composition. The volatile products formed from the pyrolysis can be oxidized in the gas phase. The following homogeneous gas phase reactions were considered (Petersen and Werther, 2005):

(a1) $CO + \frac{1}{2}O_2 \xrightarrow{Kg1} CO_2$ $R_{g1} = \varepsilon \cdot k_{g1} \cdot [CO][H_2O]^{0.5}[O_2]^{0.25}$ (g2) $H_2 + \frac{1}{2} O_2 \xrightarrow{Kg2} H_2O$ $\mathbf{R}_{p2} = \mathbf{\epsilon} \cdot \mathbf{k}_{p2} \cdot [\mathbf{H}_2] [\mathbf{O}_2]$ (g3) $CH_4 + 3/2 O_2 \xrightarrow{Kg3} CO + 2H_2O$ $\mathbf{R}_{g_3} = \varepsilon \cdot k_{g_3} \mathbf{T}_g \cdot [\mathbf{CH}_4]^{0.5} [\mathbf{O}_2]$ (g4) $C_2H_6 + 5/2 O_2 \xrightarrow{Kg4} 2CO + 3H_2O$ $\mathbf{R}_{g4} = \varepsilon \cdot k_{g4} \cdot \mathbf{T}_{g} \cdot [\mathbf{C}_{2}\mathbf{H}_{6}][\mathbf{O}_{2}]$ (g5) $C_6H_6 + 3O_2 \xrightarrow{Kg5} 6CO + 3H_2$ $R_{g5} = \varepsilon \cdot k_{g5} [TAR][O_2]$

The water gas shift reaction is active in the pyrolysis and the drying zone as well and is modeled as follows:

(wgs)
$$CO + H_2O \leftrightarrow H_2 + CO_2$$

 $R_{wg} = \varepsilon \cdot k_{wg} \left\{ [CO][H_2O] - \frac{[CO_2][H_2]}{K_{wg,eq}} \right\}$
 $k_{wg} = 2.78 \cdot 10^3 \cdot exp(-1513/T_g) \text{ m}^3/(s \cdot kmole)$
 $K_{wg,eq} = 0.0265 \cdot exp(3966/T_g)$

he char derived from pyrolysis is oxidized with the supplied air:

(s1)
$$C + 1/2O_2 \rightarrow 2CO$$

In the gasification zone the following reactions of the char were considered in the model:
(s2) $C + CO_2 \rightarrow 2CO$ (s3) $C + 2H_2 \rightarrow CH_4$ (s4) $C + H_2O \rightarrow H_2 + CO$
The ash layer was assumed to remain intact on the particles. So, the shrinking unreacted core model was
assumed for all the heterogeneous reaction of the char with the following expression for the reaction rate:

$$R_{si}(kg_{c}/m^{3} \cdot s) = \frac{\rho_{gl}}{\frac{1}{k_{diff,gl}} + \frac{1}{k_{ash,gl}} \left(\frac{1}{\zeta} - 1\right) + \frac{1}{k_{si} \cdot \zeta^{2}}} \cdot \frac{M_{c}}{\nu_{gl,sl}M_{gl}} \cdot A_{sg} \qquad gl = O_{2}, CO_{2}, H_{2}, H_{2}O_{2}, H_{2}O_{2}, H_{2}, H_{2}O_{2}, H_{2}O_$$

The resistances in the denominator represent diffusion through the gaseous film, diffusion through the ash layer and surface reaction. The ash diffusion rate kash depends on both the gas diffusivity and the voidage of the ash layer and, generally, can be roughly estimated by the correlation suggested by Wen and Chaung (1979). The kinetic parameters for the char oxidation and the char gasification with carbon dioxide and steam are derived from the data determined by Nowicki et al. (2010) for char obtained by pyrolysis of

sewage sludge having similar composition to that of the sample used in this study. Hydrogasification is generally negligible under atmospheric pressure and its rate is assumed to be three orders of magnitude smaller than the carbon dioxide gasification rate. Literature correlations are used for the gas/solid heat transfer and the mass transfer coefficients (Hobbs et al., 1992).

2.3 Simulation

The model was implemented in the Simulink® (Matlab®) simulation platform with a view to easy accessibility. The reactor was divided into many small cylindrical cells, whose cross sections coincide with the reactor cross section, while the height Δz can be variable. The model equations were applied to each cell considered as a continuous stirred reactor. To solve the differential equations, the implicit ode23s solver was used with variable time step and a relative tolerance of 10^{-3} . Based on the boundary and initial conditions, the model computes the transient profiles of temperature, velocity and composition of solid and gas phases along the gasifier.

2.4 Experimental setup

The model was validated with the experimental data published by Seggiani et al. (2011, 2012) derived from tests performed in a pilot-scale plant operating at atmospheric pressure whose schematic flowsheet is reported in Figure 1. The core of the plant is a stainless steel cylindrical reactor with an internal diameter of 165 mm and a height of 2m. Temperature profiles along the gasifier bed are measured by eight K-type thermocouples, disposed 70 mm apart one from the other above the grate. The gasifier is externally covered with an isolation blanket to reduce heat loss. The sewage sludge pellets are continuously fed at the top of the gasifier at a level located 1 m above the grate by a variable-speed screw feeder. The incoming air flow rate was automatically controlled. The product gas was conveyed through a cleaning/cooling system. The clean gas composition was analyzed by a gas chromatograph and mass spectrometer (Agilent 5975C series GC/MSD System). The equivalence ratio (ER) was calculated as ratio between the quantity of actual air and the stoichiometric air required for complete combustion. C, H and S contents of the feedstock were considered to evaluate the amount of stoichiometric air.

3. Results and discussion

Figure 2a shows the experimental temperature profiles measured at various locations along the gasifier. As shown, because the fuel bed was ignited by an igniter located at few centimetres above the grate, the temperature at this location rose first up to the peak value of 1450 K and then declined because the oxidation front propagated upward from this location to the top of the fuel bed. This is due to the fact that the combustion rate was significantly higher than the actual solid rate along the gasifier. When the time reached the range of 200-210 min, the bed was in steady state condition. The peak temperature stayed at the distance of 50 cm above the grate, after the flame front reached this height. As a result, at the steady state all the main processes such as drying, pyrolysis and gasification/combustion took place at the top of gasifier where all the char was consumed. Below this height, a thick ash layer formed above the grate (0.3 kg of ash were produced for kg of sewage sludge gasified). In this zone the temperatures dropped because of cold gas that rose. From an operational point of view, the feeding rate should be increased in order to move the oxidation front downward from the top to the bottom near the grate and, at the same time, the frequency of accumulated ash discharge at the grate should be increased to maintain constant the bed height. In fact, experimentally, after ash discharge, a rapid temperature rise was observed and, as expected, a slight reduction in the upper part, due to bed movement.

Simulations were carried out with the input parameters listed in Table 1 corresponding to the operating conditions of the gasification experiments performed and to the analyses of the used sewage sludge sample. In an updraft gasifier the composition of producer gas depends strongly on the product composition of the pyrolysis reaction. Consequently, in the model the producer gas composition can be mainly influenced by changing the splitting factors in the pyrolysis reaction.

Parameter	value	Analyses of sewage sludge				
Ts ⁱⁿ , Tair ⁱⁿ	298.15 K	Proximate analysis, wt %		Ultimate analysis, daf wt %		
dp	0.01 m	Moisture	20	С	51.2	
ER	0.25	Volatile matter	44	Н	8.2	
Wss	3.5 kg/h	Ash	30	N	7.1	
Н	0.6 m	Fixed carbon	6	S	1.7	
3	0.27 ^a			0	31.8	

Table 1. Input parameters for the simulation of the gasifier and the sewage sludge analyses.

^a valuated by the measured values of the absolute and apparent (bed) densities.

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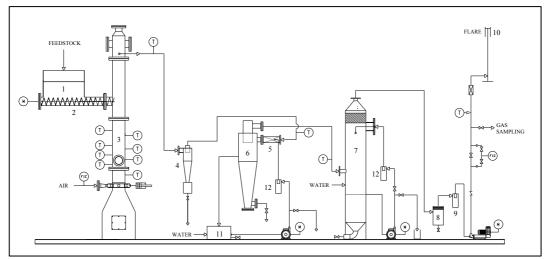


Figure 1: Schematic flowsheet of the gasification pilot plant: (1) feed hopper, (2) screw feeder, (3) gasifier, (4) cyclone, (5) venture scrubber, (6) wet cyclone, (7) wet scrubber, (8) packed-bed filter, (9) paper filter, (10) flare, (11) water tank, (12) water filter.

Starting from an initial temperature profile similar to the experimental and using the following splitting factors: $\xi_{NH3} = 0.33$ (Petersen and Werther, 2005); $\xi_{CO} = 0.01$; $\xi_{CO2} = 0.18$; $\xi_{CH4} = 0.14$; $\xi_{H2} = 0.04$, the predicted profiles (Fig. 2b) show the same experimentally observed dynamic behaviour of the gasifier with the combustion front which moves upwards. The steady-state predicted temperatures at the bottom are lower than the experimental ones, probably because in the model the heat transfer across the bed by conduction was not considered. The splitting factors reported above allowed the best fit between the predicted and the experimental gas composition as shown in the Figure 3. Also the predicted specific dry gas rate calculated per weight of feedstock is in close agreement with the experimental data. It was not possible to compare the specific production of tar with the experimental value because the latter was not determined during the tests.

4. Conclusions

A one-dimensional unsteady state mathematical model for a fixed-bed updraft gasifier operated with sewage sludge was developed and implemented on Matlab. The simulation results were compared with measurements derived from gasification runs performed on a pilot updraft gasifier. Good agreement was achieved between predictions and experimental measurements for the dynamic axial temperature profiles and the composition of the product gas.

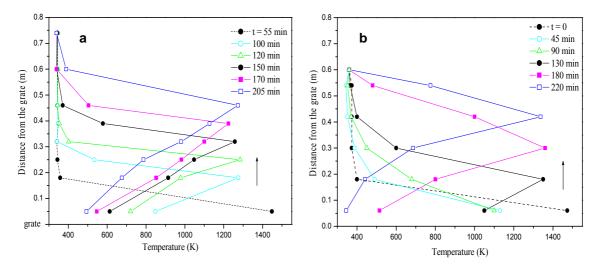


Figure 2: (a) Experimental temperature profiles and (b) calculated axial solid temperature profiles at various stages inside the bed at ER = 0.25.

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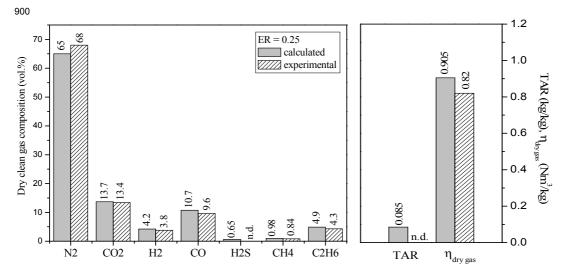


Figure 3: Comparison between the simulation predictions with the experimental data.

The model can be used as a tool to study the effect of process parameters, such as particle mean diameter and composition of sewage sludge, equivalent ratio, composition and temperature of the gasifying agent (air or air + steam) on the yield and composition of the produced gas, in view of reactor design and optimization in relation also to its dynamic behaviour.

Nomenclature

-										
	А	surface area (m ²)		Greek letters						
	Cp	specific heat (J/(kg·K)	α_1	stoichiometric coefficient of the char						
	d _p	particle size (m)	ΔH	reaction enthalpy (J/kmol)						
	ER	equivalent ratio (-)	3	bed void fraction						
	k	^{diff} gas or ash film diffusion constant (m/s)		fraction of the particle radius occupied by unreacted char						
	k _{diff} k _{ash}									
	Μ	molecular weight (kg/kmol)	ξ	splitting factor						
	N _{Rg} number of gas-phase reactions		v _{ik}	stoichiometric coefficient of the species i in the reaction k						
	Р	pressure (atm)								
	Q			mass concentration for gas (kg/m ³) and apparent density for solid (kg/m ³ _{bed})						
	R									
	R	universal gas constant		Subscripts						
	Т	temperature (K)	g	gas						
	t	time (s)	S	solid						
	u	velocity (m/s)	W	wall						
	z	coordinate in axial direction (m)								

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