

A MATHEMATICAL MODEL FOR STRATIFIED DOWNDRAFT GASIFIERS

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INTRODUCTION

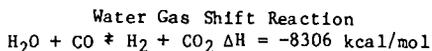
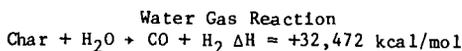
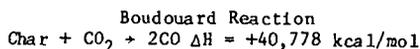
The downdraft gasifier originating from World War II Swedish designs has proven to be successful in generating a clean product gas when operated in an air blown mode. Such gas producers are useful for generating an essentially tar free boiler gas or engine fuel from renewable resources such as wood and agricultural waste. Recently, a new generation of stratified downdraft gasifiers (1, 2) has been studied. A successful model of this type of gasification process should be able to clearly show the interdependency of operating variables in order to optimize both cost of gasifier and performance. Such a process model would be useful in determining the proper gasification conditions when input conditions or design parameters change.

Figure 1 shows the important features of the gasifier. Biomass fuel and oxidizer are fed concurrently to the top of the gas generator where pyrolysis of the fuel takes place. The pyrolysis reaction is driven by heat transfer from the gas and hot char bed below. As the fresh solid is heated it dries and devolatilizes. The volatiles evolved contain combustible species which react with oxygen/air to produce heat, CO, CO₂, H₂, H₂O and light hydrocarbons. During pyrolysis, the gas and solid are at vastly different temperatures because pyrolysis cools the solid while oxidation heats the gas. (At the end of pyrolysis the gas may be more than 500K hotter than the solid.) In this zone of the reactor, about 80% to 90% of the solid weight loss occurs.

Once oxygen is consumed and pyrolysis is completed, reduction of char by CO₂ and H₂O can occur in the gasification zone. The reactions occurring are endothermic so that the gas and solid temperatures fall as carbon conversion proceeds. The reactions tend to quit at about 1000K due to kinetic limitations.

In the steady-state operation of the downdraft gasifier, a specific oxygen to fuel ratio exists for a given feedstock and carbon conversion level. In practice it is found that gasifier throughput does not affect the required O₂/fuel ratio and the product gas composition for a sufficiently deep char bed. Also, it is found that the majority of hydrocarbons are destroyed in the pyrolysis zone. These data suggest that the pyrolysis and gasification zones are to a good approximation separate and that the whole char bed in downdraft gasifiers is not truly active.

In the char gasification zone three reactions dominate (neglecting the cracking of residual tars and hydrocarbon gases from the pyrolysis zone):



The kinetics and thermodynamics of these reactions determine the conversion of char to gas and the subsequent gas composition at any point in the char gasification zone.

In the reaction scheme, the water-gas and Boudouard reactions are coupled by the shift reaction. Therefore, only two of these reactions can be considered to be truly independent. The water-gas shift reaction is fairly rapid over carbon surfaces at gasification temperatures and is assumed to be in equilibrium in this investigation. In our model we have assumed that Edrich et al. (3) kinetics for the Boudouard reaction over ponderosa pine charcoal approximates the carbon reduction reaction occurring in the gasifier. Since the activation energy for carbon reduction by CO_2 is about 35 kcal, kinetics in error by a factor of 2 will be equivalent to a 50°C offset. This offset is within the accuracy of data available for bed temperature. At atmospheric pressure, this reaction sequence should adequately describe the kinetic processes. At elevated pressure, methane forming kinetics should probably be considered. For char particles with minor dimensions up to $3/4$ inch, Edrich et al. (3) also show that intraparticle mass transfer is not important. Therefore, the same rate expression for char gasification applies regardless of particle size (if less than $3/4$ inch).

The reactor design conditions which affect the char gasification zone include initial conditions, such as char and gas temperatures, flow rate and composition of the incoming gas, and gasifier parameters, such as char gasification kinetics, cross-sectional area of reactor, heat transfer from the gas to the solids, and the density and void fraction of the char. An adequate model must account for changes in these initial conditions and parameters.

To date the most extensive modelling of the char zone of the stratified downdraft gasifier has been developed by Reed (1). Reed's model of the char gasification zone assumes equal molar feed rates of CO_2 and carbon (char). This zone is assumed to be adiabatic, yielding a change in temperature of about 24°K per 1% of reaction of carbon. Coupling the temperature change to the kinetics of the Boudouard reaction then yields the conversion of carbon and temperature of the reaction versus time and position (depending on feed rate). The model gives a good first approximation of the gasifier behavior leading the way towards the use of theory for practical predictions.

MODEL FORMULATION

The overall gasifier model consists of two parts; these are a pyrolysis model and a gasification model. The pyrolysis model is used to provide a starting gas composition, flow rate, and temperature for the char gasification zone. To initiate the modelling, the air/fuel or O_2 /fuel ratio, feed ultimate and proximate analysis and a methane leakage from the gasifier are specified. The model generates pyrolysis gas composition and temperature along with carbon conversion gas composition and temperature along the char bed length.

Pyrolysis Model

Biomass is assumed to be artificially composed of fixed carbon (char) and volatile matter. Upon pyrolysis, for biomass under downdraft gasifier conditions, the char yield is assumed to be equal to that from the proximate yield. The char is treated as pure carbon. With the specification of an air or O_2 /fuel ratio and feed composition, an adiabatic reaction calculation around the pyrolysis zone will yield temperature, gas composition and flow rate. It is further assumed that any methane escaping pyrolysis is not cracked in the char bed. Therefore, the mass and energy balance around the pyrolysis zone allows for the methane leakage specified as a model input.

In order to calculate the adiabatic flame temperature of the pyrolysis gas, when it is oxidized by the air or oxygen, first the energy released by the combustion is determined.

$$\Delta H_{298} = \text{HHV} - \Delta H_{\text{combustion}}$$

where ΔH_{298} is the energy released from the pyrolysis and partial combustion assuming N_2 , CO , CO_2 , H_2 , H_2O , CH_4 , and char are the only products, HHV is the high heating value of the biomass (calculated by the ITG method), and $\Delta H_{\text{combustion}}$ is the sum of the moles of the products of pyrolysis times their heats of combustion. In the model predictions presented below, a typical biomass composition of 51 percent carbon, 6 percent hydrogen and 43 percent oxygen by weight was assumed for the material balance calculation.

The adiabatic flame temperature can then be determined by the following equation

$$\int_{T_{298}}^{T_{\text{flame}}} \sum m_i C_{p_i} = \Delta H_{298}$$

In this model an integral average value of C_{p_i} for each of the gas constituents is utilized. The calculated adiabatic flame temperature is then used to determine the correct K_p and gas composition in a second iteration. Since the flame temperature varies little with changes in K_p , only two iterations are necessary for accurate gas composition and adiabatic flame temperature predictions. Specifying the amount of fixed carbon yielded from the biomass and the oxygen to fuel ratio gives a unique gas composition and temperature.

Char Gasification Model

The char gasification model described below assumes that the char gasification zone is adiabatic and, as in the pyrolysis zone, the water gas shift reaction is at equilibrium. Char gasification kinetics are employed to compute the conversion/length profile. Heat balances on the gas and solid are used to determine temperature profiles. Material balances written for gas and char in the reactor assume plug flow; however, the gas and char move at different rates down the reactor. The fractional conversion of the char, X , is defined as follows:

$$X = (\dot{m}_c(0) - \dot{m}_c(z)) / \dot{m}_c(0)$$

where $\dot{m}_c(0)$ = molar flow rate of carbon at top of gasification zone, and $\dot{m}_c(z)$ = molar flow rate of carbon at position "z" in the gasification zone. The carbon mass balance is then:

$$\dot{m}_c(0) dX/dz = r_c S$$

where X is the fractional conversion of the char, z is the distance down the reactor, r_c is the rate of conversion of in moles char/min, S is the cross sectional area of the reactor, and $\dot{m}_c(0)$ is the char feed rate in moles char/min. The rate is computed from kinetic data.

For the Boudouard reaction:

$$-r_c = (k_1 \cdot \text{PCO}_2) / (1 + k_2 \cdot \text{PCO})$$

$$k_1 = \exp(-E_1/RT + 12.3091)$$

$$k_2 = \exp(-E_2/RT - 28.4295)$$

where r_c is in units of l/min, $E_1 = 43870 - 19811/T_p$ (pretreatment) cal/mol, $E_2 = -67,300$ cal/mol and PCO and PCO_2 are partial pressures of CO and CO_2 respectively. The pretreatment temperature is the temperature at which the biomass is pyrolyzed. In this model it is assumed to be 1000K. For the purpose of this model, the bed voidage and particle size are assumed constant. Shift kinetics are assumed to be rapid. Thus, the gas composition is brought to a water gas shift equilibrium at each position in the reactor. To account for kinetics the equilibrium constant is displaced from the gas temperature by 50°C.

The energy balance includes individual equations for the char, and one for the gas phase. In the gas phase:

$$\Sigma m_g c_p \frac{dT_g}{dz} = h \cdot A_p (T_s - T_g) \rho (1 - \epsilon)$$

where m_g is the mass flow rate of the gas, c_p is the heat capacity of the gas, T_g is the gas temperature, h is the heat transfer coefficient between the gas and the char, A_p is the surface area per gram char, T_s is the char temperature. ρ is the char density and ϵ is the void fraction in the bed.

For the solid phase

$$\Sigma m_s c_p \frac{dT_s}{dz} = - \Sigma m_g c_p \frac{dT_g}{dz} - (\dot{m}_c(0) \cdot \frac{dX}{dz} \cdot \Delta H_B + \dot{m}_{H_2O}(0) \frac{dY}{dz} \cdot \Delta H_{WGS})$$

where X is the conversion of char, H_B is the heat of reaction for the Boudouard, Y is the conversion of steam to hydrogen, and H_{WGS} is the heat of reaction for the water gas shift reaction. The mass and energy balances are coupled and solved using a Runge Kutta integration routine in an interactive mode.

The model results are very dependent on initial conditions, including the input from the pyrolysis model calculations of temperature and composition of the gas. The average temperature of the solid is not known exactly but is assumed to be somewhere between the flame temperature and the pyrolysis front temperature. The solid temperature is not critical, since the heat transfer coefficient is large and the heat capacity of the solid phase is small relative to the gas phase.

The heat transfer coefficient in the energy balance has been calculated by an empirical correlation of Satterfield (4) for fixed bed reactors. The model needs the area to volume ratio of the feedstock to calculate the heat transfer coefficient, h , and the particle area to weight ratio, A_p .

EXPERIMENTAL DATA

To compare the prediction of the model with experimental gasifier results, a quartz tube gasifier 54 mm outer diameter, shown in Fig. 2, was employed. A type K 1/16-in. thermocouple was used for temperature measurement through the pyrolysis and gasification zones. A 1/16-in. 304 SS tube was placed directly alongside the thermocouple, through which gas samples were pulled. A 10 cc syringe (+ needle) was used to evacuate the tube and to take the sample. Gas analysis was done with a Carle #111H gas chromatograph, with a hydrogen transfer tube and a ten ft Carbosieve column. Integration of analysis was performed with a Varian # CDS111 integrator.

Two samples were taken for each level measured. Once a steady state condition in the gasifier was achieved, the probes were inserted to the specified level and the gas sampling temperature recording procedure begun. The probes were then moved at 2 cm intervals up through the bed until the temperature read below gasification pyrolysis temperatures (100°C). The time interval in between each sample was approximately 1 minute.

RESULTS

Table 1 presents results of the pyrolysis material and energy balance model. The adiabatic flame temperatures of the pyrolysis products, assuming fractions of fixed carbon from 0.05 to 0.20 when burned with various ratios of O_2 /fuel has been calculated. The model also yields the gas composition at the end of pyrolysis for each fixed carbon and O_2 /fuel ratio. The gas temperature and composition is then input into the gasification model. For predictions of the laboratory data, the fixed carbon is assumed to be 15% and the O_2 /fuel ratio is set at 0.45. For the oxygen runs the O_2 /fuel ratio is assumed to be 0.40. The results presented yield varying char loss through the grate. An alternate calculation is to iterate on the air/fuel ratio to consume a specified amount of fixed carbon.

Table 1. Pyrolysis Model Calculations

Feed Gas	O_2 /Fuel	Fraction Fixed Carbon	Adiabatic Flame Temperature (K)
Air (O_2)	0.4	0.05	575 (888)
		0.10	764 (1182)
		0.15	955 (1475)
		0.20	1146 (1765)
	0.45	0.05	745 (1201)
		0.10	924 (1490)
		0.15	1104 (1775)
		0.20	1282 (2055)
	0.50	0.05	897 (1504)
		0.10	1067 (1785)
		0.15	1236 (2061)
		0.20	1403 (2330)

Figure 3 shows the model predictions of the char and gas phase temperature profiles through the gasification zone for air gasification. The solid phase is represented by the solid line, the gaseous phase is represented by the dotted line and the experimental data are represented by stars. Excellent agreement with the data is observed throughout the char gasification zone, with the exception of the data point at the grate. This discrepancy is caused by heat loss (conduction and radiation) at the grate, resulting in lower temperature measurements than expected. In a reactor with a layer of ceramic balls above the grate it would be expected that heat loss would not be important.

Figure 4 shows predictions and experimental data of the CO/CO_2 ratio down the reactor. The agreement between model predictions and experimental data is good

confirmation of the model. Since no adjustable parameters were input into the model to make the temperature profile and CO/CO₂ ratio predictions, the model appears successful at simulating laboratory conditions.

The effect of varying throughput on char conversion is shown in Fig. 5. In this figure, the result of inputting into the model ten times normal, normal, and one tenth normal air throughput is illustrated. Quantitatively, after the solid and gas have come to the same temperature, the conversion of char for a given distance is linearly dependent on the throughput. Although an increase in throughput increases the heat transfer from the gas to the solid, the net effect on char conversion, as yielded by model calculations, is the same char conversion for equivalent residence times, regardless of throughput. Increasing the surface area/volume ratio for the feedstock also increases heat transfer from gas to char, but again no significant difference in conversion occurs for various ratios, after the gas and solid temperatures approach the same point.

Figure 5 also shows the char conversion for a throughput consisting of oxygen instead of air. An interesting outcome from using oxygen in the model calculations is that the temperature of the char only rises about 50K above the peak temperature of the air gasification case, as depicted in Fig. 6. This is in spite of the initial gas temperature of the oxygen run of 1750K, compared to 1400K for the air case. Similar results have been observed in the laboratory for the oxygen gasifier. The reason for this phenomenon is the buffering effect of the endothermic gasification reactions which increase their rates at higher temperatures, thus converting greater amounts of sensible heat to chemical energy. The end result then is not higher temperatures in the reactor but higher conversion of the char in the gasification zone.

CONCLUSIONS

- (1) A pyrolysis model has been developed which yields gas temperature and composition for both air and oxygen gasification. The results of this model are then input into a separate char gasification model.
- (2) A char gasification model has been developed which utilizes no adjustable parameters to predict design parameters and gasifier process conditions.
- (3) The two models yield realistic temperature profiles of the solid and gas phases down the reactor. Predictions compare very well with laboratory data.
- (4) The CO/CO₂ ratio predicted agree well with laboratory data.
- (5) The model shows an essentially linear correlation between throughput and char conversion for a given reactor length.
- (6) The model predicts equivalent conversions of char for various surface to volume ratios of the same feedstock.
- (7) The model demonstrates the buffering effect of the endothermic gasification reactions in keeping down the char temperature in an oxygen gasifier.

RECOMMENDATIONS

- (1) A model should be incorporated to give the residence time and integral average temperature of the char after pyrolysis. This addition would allow determinations of the appropriate reactor length for complete gasification, and remove the estimation of initial particle temperature in the char gasification zone.

- (2) Experimental data should be taken with various gasifier conditions and designs to check model predictions and assumptions.

ACKNOWLEDGEMENTS

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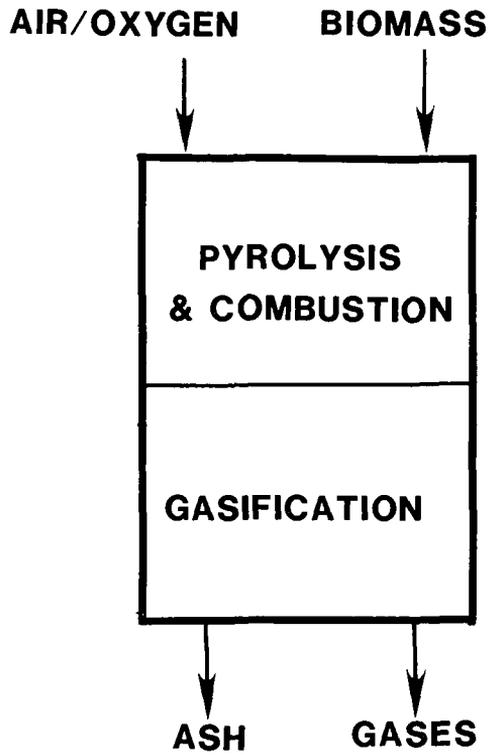


Figure 1. Stratified Downdraft Gasifier.

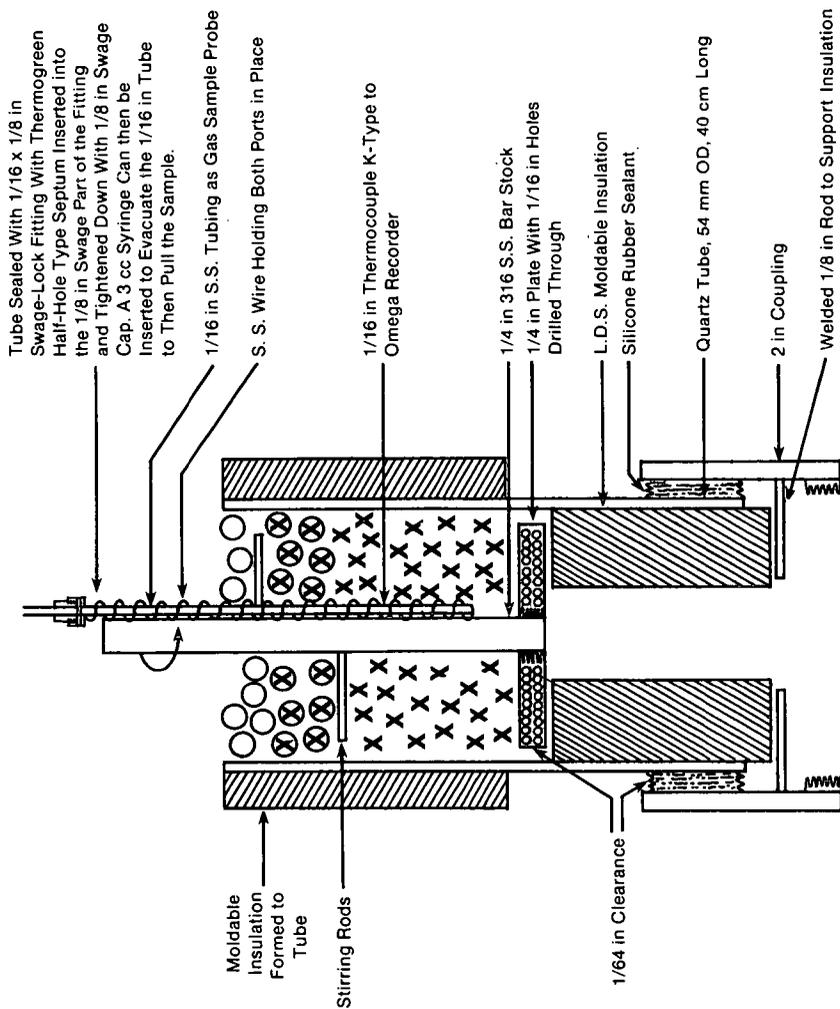


Figure 2. Quartz Tube Gasifier and Measurement Apparatus.

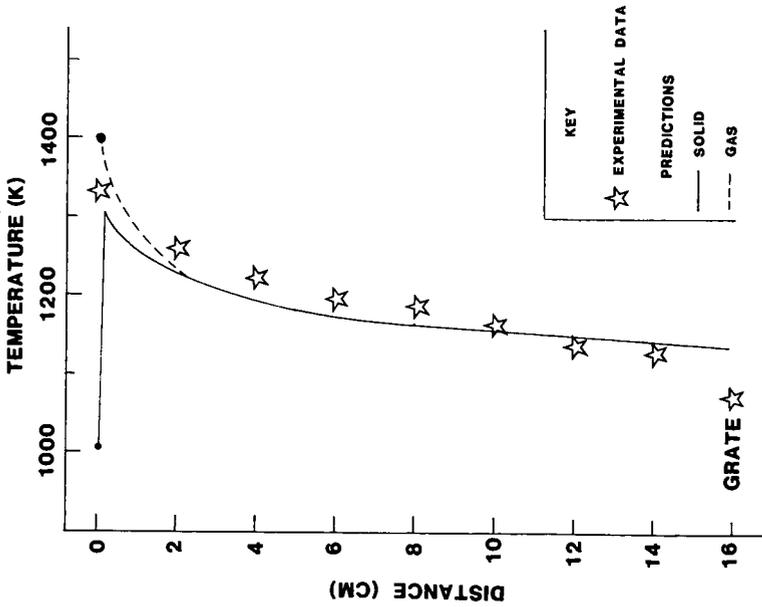


Figure 3. Char Gasification Zone Solid and Gas Temperature Predictions and Experimental Data for Air Gasifier with 1/4-in. Wood Chips.

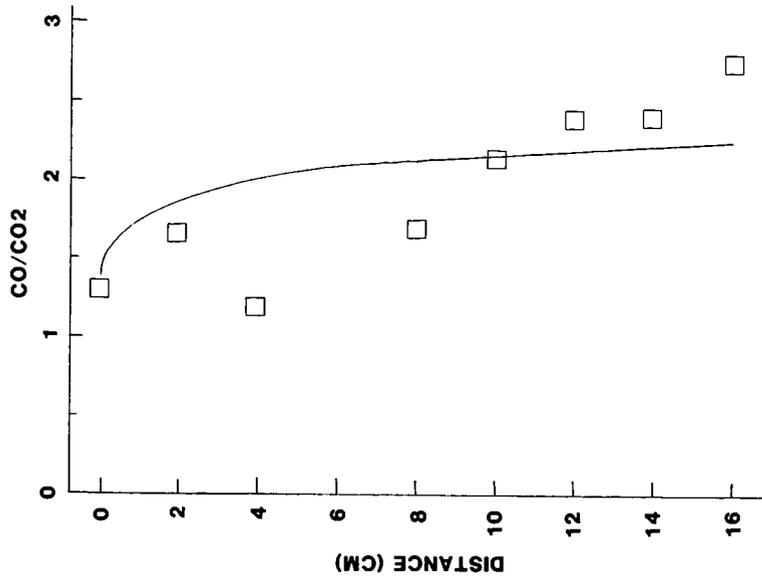


Figure 4. Char Gasification Zone CO/CO₂ Prediction and Experimental Data for Air Gasifier with 1/4-in. Wood Chips.

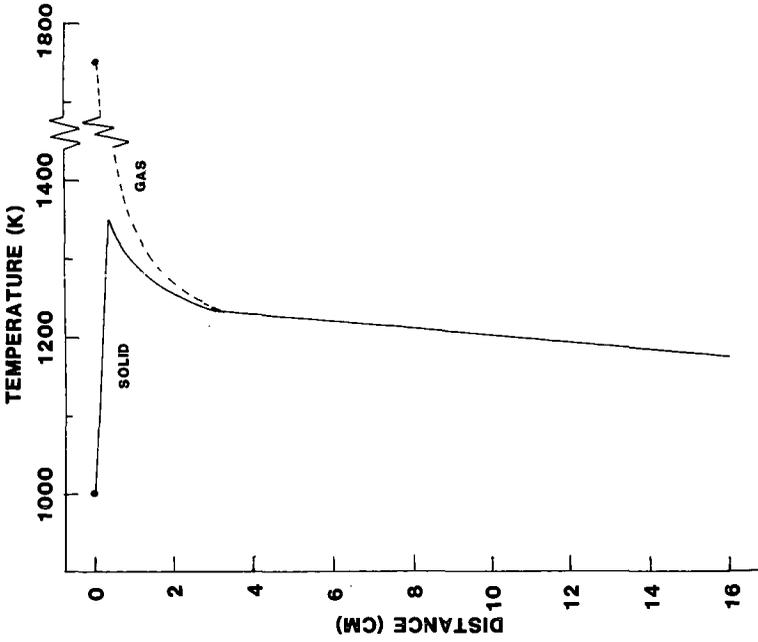


Figure 6. Char Gasification Zone Solid and Gas Temperature Predictions for Oxygen Gasifier with 1/4-in. Wood Chips.

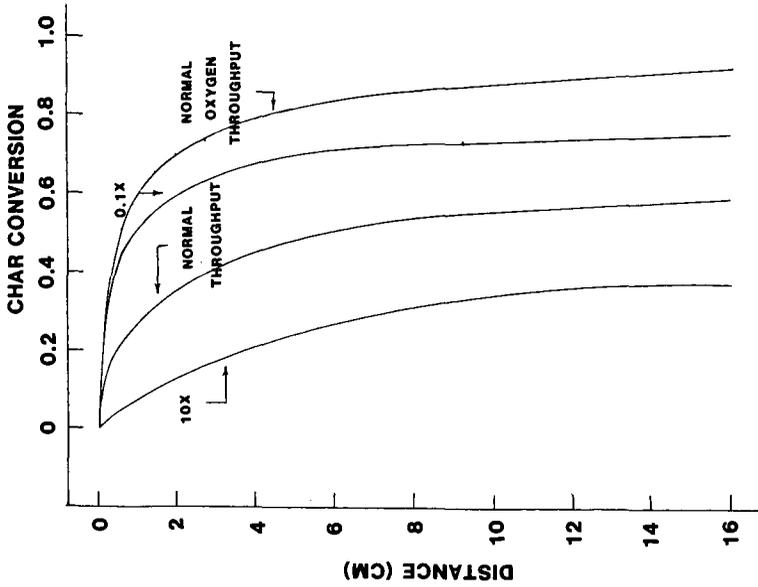


Figure 5. Char Gasification Zone Fractional Char Conversion for Various Air and Oxygen Throughputs.