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Model Development of UCG and Calorific Value Maintenance via Sliding Mode Control

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***Abstract*—The design of underground coal gasification (UCG) process is a difficult task, especially if its performance needs to be compared with surface gasification, because in UCG there is a lack of direct control to many important parameters. In this work a nonlinear time domain model of UCG is formulated by incorporating some assumptions in already existing models of [1] and [2]. The input of the model is molar flow rate of inlet gas (mixture of Air and steam), and output is the calorific value of exit gas. In order to keep the calorific value at a desired value in the presence of external disturbance, the model is used in a closed loop configuration with a sliding mode controller (SMC).**

I. Introduction

To address the short fall of electricity generation in Pakistan, UCG Thar has launched the project of underground coal gasification (UCG) in Thar coal field. Thar coalfield is the biggest coalfield of Pakistan, located in southeastern corner of Sindh province of Pakistan and contains over 175 billion tons of lignite coal [3]. UCG consists of a pair of wells: injection and production wells, which are drilled from the surface to the coal seam. Gasification occurs by injecting the oxidants (air/oxygen (O_2) and steam (H_2O) in to the injection well. The injected gas mixture reacts chemically with coal to produce synthesis gas (a mixture of CO and H_2), which can be used as a fuel for combined cycle turbines (CCT) for electricity generation or as a chemical feedstock [4], [5] and [6].

The process of UCG has a lot of advantages over conventional mining e.g. it allows access to more coal resources than economically recoverable by traditional technologies, and it becomes the only choice if the coal is not minable. Despite of the advantages, there are also some limitations to the commercialization of UCG e.g. the product gas from UCG has less heating value (88.23 to 264.70 KJ/moles [5]) as compared to surface gasification. Two indicators for measuring the success of UCG process are: Calorific value of exit gas and resource recovery of coal seam for a given configuration of injection and production wells.[7]. Four different types of mathematical models of UCG are found in the literature: channel model, packed bed model, coal block model and process model [4]. In channel model, injection and production wells are physically linked by a horizontal borehole. The coal is gasified at the perimeter of the channel. This type of method is used for the high rank coal which has very poor permeability, e.g. anthracite. Magnani et al., [8] and [9] developed two channel models of UCG. Packed bed modeling technique is used for low and medium rank coals, e.g. lignite and sub-bituminous, these coal types have relatively higher permeability than anthracite. Winslow et al., [1], Thorsness et al., [2], Khadse et al., [5] and Perkins et al., [7] modeled UCG process as a packed bed, all of these models represent the process in time and at least one space dimension. In coal block model coal seam is considered as a wet slab of coal, which is initially dried and then gasified. Perkins et al., [10] has considered coal block model for simulation. Process models calculate the cavity growth of the UCG reactor with time in a three dimensional (3D) space, Beizen al., [11] considered this type of modeling. The objective of all of these models is to evaluate a potential UCG site.

In literature there is no evidence of model based control of UCG process, the control of process mainly includes the work of Karol Kostur et al., [12] and [13]. The authors deployed Proportional Integral (PI) control scheme on laboratory scale UCG rig, in which volumetric flows and synthesis gas (syngas) temperature are controlled.

In this research work emphasis has been laid on model based control of UCG process. Section II discusses the evolution of a time domain model of UCG and model validation, Section III explains the implementation of SMC algorithm on the developed model and the research work is concluded in Section IV.

II. Mathematical Model

This Section briefly discusses all the steps taken in order to formulate a time domain model of UCG reactor.

A. 1-D Packed Bed Model

The approach of simulating UCG process as a packed bed reactor is very famous. The 1-D packed bed models of [1], [2] and [5] is used in the current work. Some important characteristics and assumptions considered in the model are as follows.

- Solid phase consists of: coal and char.
- There are eight gas species considered in the model: CO, CO_2, H_2, CH_4, H_2O, O_2, N_2 and tar (a pseudo specie used to close the stoichiometry of coal pyrolysis [2]).
- The gas pressure is considered constant, because there is a very little pressure drop between the inlet and outlet wells [5].
- For the simplicity purpose, the porosity of the coal bed is taken constant.

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- Three reactions are considered in the model: coal pyrolysis, char oxidation and steam gasification.

The mathematical model consists of gas and solid phase equations

1) Gas Balance Equation:

$$\phi \frac{\partial}{\partial t}(c_i) = -\frac{\partial}{\partial x}(c_i v) + \sum_{j=1}^{3} a_{ij} r_j \quad (1)$$

where ϕ is the porosity of coal bed, v the gas velocity (cm/sec), c_i the concentration of ith gas specie (moles/cm^3), a_{ij} the stoichiometric coefficient of ith gas specie in jth chemical reaction, the coefficients are positive for the products and negative for the reactants, and r_j the rate of jth chemical reaction (moles/cm^3/sec).

2) Mass Balance For Solid:

$$\frac{\partial \rho_i}{\partial t} = M_i \sum_{j=1}^{3} a_{s_{ij}} r_j \quad (2)$$

where ρ_i is density of the ith solid specie (g/cm^3), M_i is molecular weight of ith solid (g/mol) and $a_{s_{ij}}$ is stoichiometric coefficient of ith solid in jth reaction.

3) Solid Phase Energy Balance:

$$\begin{aligned} C_s \frac{\partial T_s}{\partial t} &= (1-\phi)\, k_s \frac{\partial^2 T_s}{\partial x^2} + h_t (T - T_s) - H_s \quad (3) \\ H_s &= \sum_{j=2}^{3} H_j r_j \end{aligned}$$

where T_s is the solid temperature (K), k_s the thermal conductivity of solid (cal/cm/sec/K), H_s the solid phase heat source (cal/cm^{3}sec), C_s the total solid phase heat capacity (cal/cm^{3}K), h_t the heat transfer coefficient (cal/cm^3/K/sec), H_j is the heat of the jth heterogeneous (solid-gas reactions) chemical reaction (cal/mol), T is the temperature (K).

For reducing the complexity of the model h_t, k_s and C_s are assigned constant values, empirical relationships for these parameters can be found in [2]. T is also a model parameter which increases the solid temperature to obtain a sufficient value of reaction rates, and it also introduces the effect of ignition in the system.

4) Chemical Reactions: Following equations represents balanced chemical reactions for coal pyrolysis, char oxidation and steam gasification reactions respectively.

$$\begin{aligned} CH_{0.912}O_{0.194} &\xrightarrow{r_1} 0.766 CH_{0.15}O_{0.02} \\ &+ 0.008 CO + 0.055 H_2O \\ &+ 0.083 H_2 + 0.044 CH_4 \\ &+ 0.058 CO_2 \\ &+ \frac{0.124}{9} (CH_{2.782})_9 \quad (4) \\ CH_{0.15}O_{0.02} + 1.028 O_2 &\xrightarrow{r_2} CO_2 + 0.075 H_2O \quad (5) \\ CH_{0.15}O_{0.02} + 0.955 H_2O &\xleftrightarrow{r_3} CO + H_2 \quad (6) \end{aligned}$$

where $CH_{0.912}O_{0.194}$, $CH_{0.15}O_{0.02}$ and $(CH_{2.782})_9$ are molecular formulas of coal, char an tar respectively.

The rates r_1, r_2 and r_3 of above chemical reactions are given in Eq (10)

$$\begin{aligned} r_1 &= 5 \frac{\rho_{coal}}{M_{coal}} \exp\left(\frac{-6039}{T_s}\right) \quad (7) \\ r_2 &= \frac{1}{\frac{1}{r_{c_2}} + \frac{1}{r_{m_2}}} \quad (8) \\ where, & \\ r_{c_2} &= \frac{9.55 \times 10^8 \rho_{char} m_{O_2} P \exp\left(\frac{-22142}{T_s}\right) T_s^{-0.5}}{M_{char}} \\ r_{m_2} &= k_y m_{O_2} \quad and \quad k_y = 0.1 h_t \\ r_3 &= \begin{cases} \frac{1}{\frac{1}{r_{c_3}} + \frac{1}{k_y m_{H_2O}}} & \text{if } A > 0 \\ \frac{1}{\frac{1}{r_{c_3}} - \frac{1}{k_y m_{CO}}} & \text{if } A \le 0 \end{cases} \quad (9) \\ where, & \\ r_{c_3} &= A \frac{r_{cc_3}}{m_{H_2O}} \\ r_{cc_3} &= \frac{\rho_{char} m_{H_2O}^2 P^2 \exp\left(5.052 - \frac{12908}{T_s}\right)}{M_{char}\left[m_6 P + \exp\left(-22.216 \frac{24880}{T_s}\right)\right]^2} \\ A &= m_{H_2O} - \frac{m_{H_2} m_{CO}}{k_{e_3}} \end{aligned}$$

where k_{e_3} the equilibrium constant for steam gasification reaction, P the gas pressure (atm), and k_y the mass transfer coefficient (moles/cm^3/sec). The mole fraction of the ith gas specie used in the above equations can be calculated as:

$$mf_i = \frac{c_i}{C_T} \quad and \quad C_T = \sum_{i=1}^{8} c_i \quad (10)$$

B. Time Domain Model

Using above assumptions the mass balance PDE's for solids and gases have been converted to ODE's.

$$\phi \frac{d}{dt}(c_i) = -\beta\,(c_i) + \sum_{j=1}^{3} a_{ij} r_j \quad (11)$$

In Eq (11) the term $\beta\,(c_i)$ approximates the spatial derivative in Eq (1), which shows that the concentration of the gas decreases when it moves through the bed. In a similar manner Eq (4) can be re-written as:

$$C_s \frac{dT_s}{dt} = \alpha\,(T_s) + h\,(T - T_s) - H_s \quad (12)$$

where $\alpha\,(T_s)$ replaces first term on the right hand side of Eq (4). Now Eq (2), Eq (11) and Eq (12) represent the UCG reactor model. The model consists of eleven first order ODE's.

1) State Space Representation: The time domain model of UCG can be written in the state pace representation as:

$$\begin{aligned} \dot{x} &= f(x,t) + gu + d\delta(t) \\ y &= h(x_4, x_5, x_6, x_7, x_8, x_9, x_{10}, x_{11}) \end{aligned} \tag{13}$$

where $x \in \Re^{11}$ is the state vector, $f : \Re^{11} \rightarrow \Re^{11}$ the nonlinear function of states, $g \in \Re^{11}$ the input vector, $u \in \Re$ the molar flow rate (moles/cm^{2}sec) of gas (a mixture of H_2O, O_2 and N_2) pumped in to the injection well is the input to the plant, $d \in \Re^{11}$ the disturbance vector, $\delta \in \Re$ the molar flow rate of water influx from the surrounding aquifers is the matched bounded disturbance $\|\delta(t)\| \leq \delta_0 > 0$, and y the calorific value of product gas (KJ/mol) is the output.

The states of the system are defined in Eq. (14).

$$X = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \\ x_6 \\ x_7 \\ x_8 \\ x_9 \\ x_{10} \\ x_{11} \end{bmatrix} = \begin{bmatrix} coal\ density \\ char\ density \\ solid\ temperature \\ concentration\ of\ CO \\ concentration\ of\ CO_2 \\ concentration\ of\ H_2 \\ concentration\ of\ CH_4 \\ concentration\ of\ tar \\ concentration\ of\ H_2O \\ concentration\ of\ O_2 \\ concentration\ of\ N_2 \end{bmatrix} \tag{14}$$

The components of vectors f, g and d, and the function $h(.)$ are given in Eq. (15)

$$f = \begin{bmatrix} M_{coal} \sum_{j=1}^{3} a_{coal,j} r_j \\ M_{char} \sum_{j=1}^{3} a_{char,j} r_j \\ \frac{1}{C_s}\left[ht(T - x_3) - H_s\right] \\ \sum_{j=1}^{3} a_{CO,j} r_j - \beta x_4 \\ \sum_{j=1}^{3} a_{CO_2,j} r_j - \beta x_5 \\ \sum_{j=1}^{3} a_{H_2,j} r_j - \beta x_6 \\ \sum_{j=1}^{3} a_{CH_4,j} r_j - \beta x_7 \\ \sum_{j=1}^{3} a_{tar,j} r_j - \beta x_8 \\ \sum_{j=1}^{3} a_{H_2O,j} r_j - \beta x_9 \\ \sum_{j=1}^{3} a_{O_2,j} r_j - \beta x_{10} \\ -\beta x_{11} \end{bmatrix}, g = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ \frac{a}{L} \\ \frac{b}{L} \\ \frac{c}{L} \end{bmatrix}, d = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ \frac{1}{L} \\ 0 \\ 0 \end{bmatrix}$$

$$h = mf_{CO} H_a + mf_{H_2} H_b + mf_{CH_4} H_c \tag{15}$$

TABLE I
INPUT PARAMETERS FOR UCG PACKED BED MODEL

Sr	Parameter	Value
1	Length of reactor	100 cm
2	Inlet gas composition	Moles
	H_2O	a = $\begin{cases} 0 & ignition \\ 0.77 & gasification \end{cases}$
	O_2	b = $\begin{cases} 0.21 & ignition \\ 0.154 & gasification \end{cases}$
	N_2	c = $\begin{cases} 0.79 & ignition \\ 0.076 & gasification \end{cases}$
	H_2O/O_2 ratio	5
3	Gas pressure	4.83 atm
4	Initial solid temperature	450 K
5	Initial coal density	0.5 g/cm^3
6	Initial char density	0 g/cm^3
7	Coal type	Sub-bituminous
9	$\alpha(T_s)$	0
10	u	a step of 2×10^{-4} moles/cm^{2}sec
11	$\delta(t)$	0

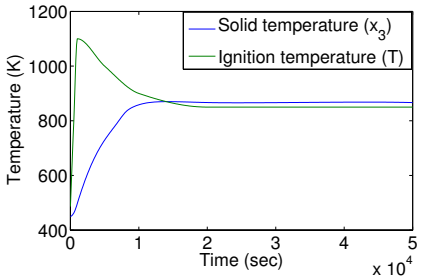

Fig. 1. Temperature profiles w.r.t time for open loop simulation

where a, b and c are percentages of H_2O, O_2 and N_2 in the inlet gas mixture, L the length of UCG reactor (cm), and H_a, H_b and H_c are heats of combustion of CO, H_2 and CH_4 (KJ/mol), which are taken from [14]. The expression for h is taken from [5].

2) Open Loop simulation: Input parameters for open loop simulations are given in Table I.

There are two modes of operation in the model: ignition and gasification. The coal seam is ignited for 1000 secs, during ignition value of ignition temperature (T) (Fig. 1) increases from 450 K to 1100 K and inlet gas is only air (Table I).

Fig. 1 represents the profiles of ignition temperature (T) and solid temperature (x_3) with time. The value of x_3 slowly approaches T due to small value of heat transfer coefficient (h_t).

Fig. 2 shows how the reaction rates are changing with time, all the reaction rates depend heavily upon x_3. Pyrolysis reaction reaches a sufficient value for $x_3 > 600K$, and both the gasification reactions attain a reasonable value for $x_3 > 800K$. Pyrolysis reaction also depends upon coal density (x_1), so it finishes around 30000 secs when the coal bed is fully consumed. Char oxidation reaction also depends upon char density (x_2) and mole fraction of O_2, so it decreases when

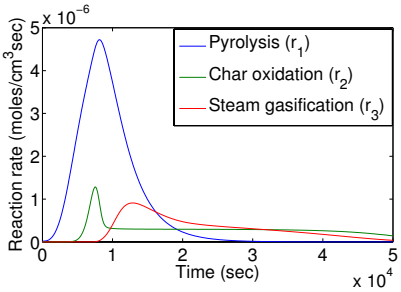

Fig. 2. Profiles of reaction rates w.r.t time for open loop simulation

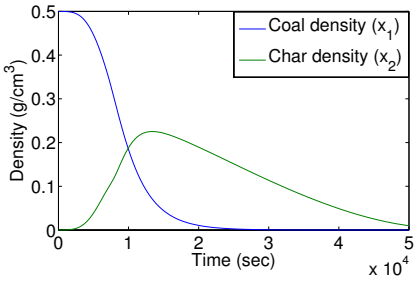

Fig. 3. Densities of coal and char w.r.t time for open loop simulation

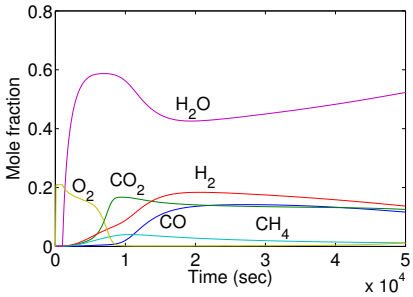

Fig. 4. Exit gas composition after open loop simulation

x_2 decreases. Steam gasification reaction also relies upon x_2 and mole fraction of H_2O.

Fig. 3 shows the trends of x_1 and x_2 with time. x_1 is consumed by the pyrolysis reaction, while x_2 increases during pyrolysis and decreases by char oxidation and steam gasification reactions.

Fig. 4 shows the composition of exit gas with time. Around 3000 secs CO, CO_2, H_2 and CH_4 start increasing due to r_1. r_2 peaks at around 8000 secs, which consumes all the O_2 and CO_2 reaches its peak value. The effect of r_3 is maximum at around 20000 secs where CO and H_2 reach their peak values and H_2O reaches its minimum value.

Fig. 5 represents calorific value (y) with time. It slowly increases to its peak value of 113.8 KJ/mol at 20000 secs, where mole fraction of CO and H_2 reach their maximum values.

3) Model Validation: Model validation is done by comparing the profiles of exit gas composition of simulated model

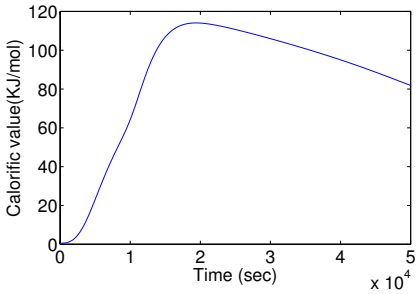

Fig. 5. Calorific value achieved at the end of the open loop simulation

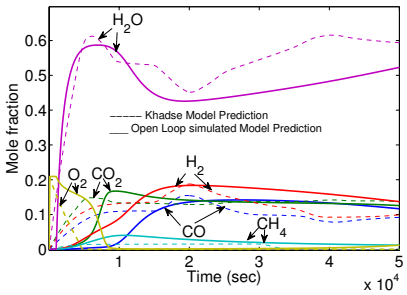

Fig. 6. Exit gas composition comparison after open loop simulation (solid lines are the result of simulated model and dotted lines represent data by [5])

with [5]. Fig. 6 shows that the trends and magnitudes of gas mole fractions are almost identical. Initially, the gases rise slowly in the simulated model due to small value of h_t, which causes slow increase in x_3. In simulated model the profiles of gas fractions are rather smooth, this is because the model contains only three reactions, however Khadse [5] has considered nine reactions. The peaks of CO and H_2 approximately occurs at the same time in both the models.

III. Controller Design

Sliding mode control (SMC) techniques provide robustness against parametric variations and external disturbances [15], so first order SMC is used to achieve following control objective.

It can be seen from the Fig. 5 that the calorific value (y) attains maximum value when CO and H_2 reach their peaks (at 20000 secs), then it starts decreasing. After this point due to low density of char, inlet gases mostly remain un-reacted, and start accumulating in the reactor, causing decrease in the mole fraction of product gases and hence y. Therefore the controller is brought in to action when CO and H_2 reach there maximum values, and it maintains the output y to the desired value (the maximum value of y), by manipulating the control effort (u). There is also a constraint on the control input: $0 \leq u \leq 3 \times 10^{-4}$ (moles/cm^{2}sec). There is a limit on the input because the compressors cannot provide very high flow rates.

To assess the robustness of the controller a matched disturbance is also considered, which is the molar flow rate of water in flux from the surrounding aquifers in situ [4], the disturbance is bounded and is shown in Fig. 7. The size

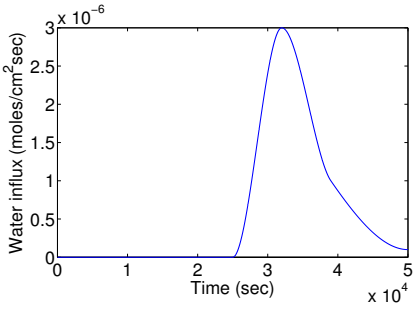

Fig. 7. Profile of water influx w.r.t time

of UCG reactor's cavity increases with the passage of time, and due to spalling of overburden rocks, water from the surrounding aquifers start entering in the cavity at 25000 secs, reaches its peak value δ_0 at 32000 secs and then keeps on decreasing with time.

For tracking problem the general form of sliding surface is given by [15].

$$s(x,t) = \left(\frac{d}{dt}+\lambda\right)^{n-1} e \tag{16}$$

For $n=0$, the sliding surface is the error dynamics of the output:

$$s(x,t) = e, \quad e = y - y_d \tag{17}$$

where y_d is constant desired calorific value.

The equivalent control method of first order SMC is applied to the system. First order sliding mode implies that the sliding mode occurs in the manifold $s=0$ [16]. The control input consists of two parts:

$$U = u_{eq} + ksgn(s) \tag{18}$$

where u_eq is continuous part of the control input, which takes the system trajectories to the sliding manifold [16], it is evaluated by making $\dot{s}=0$.

$$\begin{aligned} u_{eq} &= L\left[C_T\gamma_1 - \gamma_2\right] \\ \gamma_1 &= \frac{r_1\gamma_3 + r_3\left(H_a+H_b\right)}{\left[H_a x_4 + H_b x_6 + H_c x_7\right]} \\ \gamma_2 &= \frac{589}{2250}r_1 + \frac{11}{200}r_2 + \frac{43}{40}r_3 \\ \gamma_3 &= (0.008H_a + 0.083H_b + 0.044H_c) \end{aligned} \tag{19}$$

$ksgn(s)$ in Eq. (18) is discontinuous part of the control input, it provides robustness against the parametric variations and external disturbances, and also introduces chattering [16]. The term $sgn(s)$ is defined as:

$$sgn(s) = \begin{cases} +1 & \text{if } s>0 \\ -1 & \text{if } s<0 \end{cases} \tag{20}$$

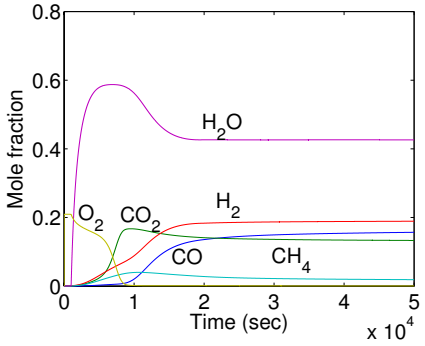

Fig. 8. Exit gas composition for closed loop system

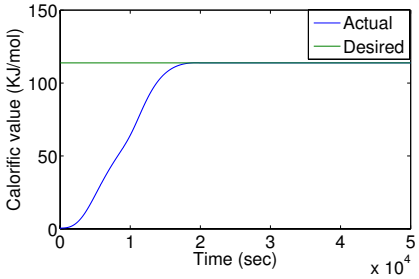

Fig. 9. Calorific value achieved at the end of closed loop simulation

The condition for existence of sliding mode and selection of gain (K) is described below.

$$\begin{aligned} Let, \quad V(s) &= \frac{1}{2}s^2 \\ \dot{V} &= s\dot{s} \\ \dot{V} &= s\frac{\psi}{L}\left[u_{eq} - U - \delta(t)\right] \\ where, \quad \psi &= \left(H_a x_4 + H_b x_6 + H_c x_7\right) \\ \dot{V} &= s\frac{\psi}{L}\left[-ksgn(s) - \delta(t)\right] \\ \dot{V} &\leq -\eta|s|, \quad k > \delta_0 + \eta, \quad \eta < k \end{aligned} \tag{21}$$

Therefore for existence of sliding mode $k > \delta_0$. The careful selection of k can provide necessary robustness with minimum chattering. When controller is switched on all the gases have non zero values of concentration, hence $\psi > 0$ in Eq.(22). The lyapunov function in Eq. (22) is positive definite, and its time derivative is negative definite, so error dynamics will converge to the sliding manifold $s=0$ in finite time [16].

A. Simulation Results

After 20000 secs the controller keeps the output at a desired value, which is shown in Fig. 9. The constant value of the output is the result of constant values of mole fractions of CO, H_2 and CH_4, shown in Fig. 8. Due to controlled molar flow rate of inlet gases, they do not unnecessarily accumulate in the reactor, this fact can be witnessed in Fig, 8.

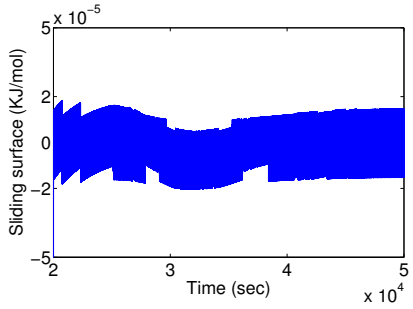

Fig. 10. Chattering in the sliding surface after controller is activated

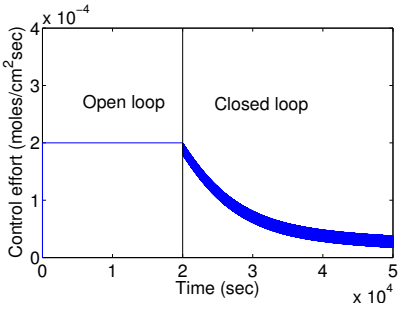

Fig. 11. Molar flow rate for open loop and closed loop systems w.r.t time.

The sliding surface is shown in the Fig. 10 after the controller is brought in the loop. The chattering is very obvious in the sliding phase. At 25000 secs the disturbance $\delta(t)$ tries to reduce the output (y), but the control shows robustness against it.

The Fig. 11 shows the controller effort after 20000 secs. To address unnecessary accumulation of inlet gases and the effect of disturbance, the controller decreases the molar flow rate of the inlet gas.

IV. Conclusion

A time domain model of UCG is formulated in this work. The model being very simple in approach and bearing a lot of assumptions, logically represents the exit gas composition of the UCG process. The proposed SMC algorithm maintains the desired calorific value of the exit gas in the presence of external disturbance i.e. water influx from the surrounding aquifers.

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