THE DEVELOPMENT OF A MATHEMATICAL MODEL TO PREDICT HEAT AND MASS TRANSFER PROCESSES ASSOCIATED WITH THE SMOKING OF A SPECIAL CIGARETTE

An Interim Report

by

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1. PURPOSE AND BACKGROUND OF THIS REPORT

1.1 Background

CHAM of North America is currently involved in the development of a mathematical model to predict heat and mass transfer processes associated with the smoking of a special cigarette being developed by R.J. Reynolds Tobacco Company. The schematics of the device are shown in Figure 1.1 and 1.2. The processes to be modelled include: air flow through the device with associated pressure drop; heterogenous and gas phase combustion in the fuel source with associated production of heat, carbon-dioxide, and carbon-monoxide; and evaporation of various flavors from the pellets in the capsule and the surrounding tobacco jacket etc. The proposed mathematical model is based on the numerical solution of the governing equations using CHAM's general purpose computational fluid-dynamics code PHOENICS [1]. Work on this contract began in May 1987 and the progress to date has been documented in CHAM's interim progress reports [2,3,4,5].

As a part of this study, the problem of flow and combustion in a single hole in the fuel source (see Figure 1.2) was analyzed at length in [4] and [5]. The schematics are shown in Figure 2. The basic reactions to be considered are:

Surface Reactions

$$C + (1 - \frac{\alpha}{2})\, O_2 \rightarrow \alpha\, CO + (1 - \alpha) CO_2 \qquad (1)$$

$$C + CO_2 \rightarrow 2CO \qquad (2)$$

Gas Phase Reaction

$$2CO + O_2 \rightarrow 2CO_2 \qquad (3)$$

The quantity α in Eqn. (1) represents the fraction of C burning to CO.

In [4], only the surface reaction (1) was considered using the reaction rate data and α as provided by Welsh and Chung [6]. Later, in [5], reactions (1), (2), and (3), were all considered using the data provided by Adomeit et.al. [7]. However, in [5], α was taken as unity — i.e., it was assumed that CO is the only product of $C + O_2$ reaction at the wall.

1.2 Purpose of this Interim Report

The purpose of this report is to document the extension of carbon burnout model presented in [5] to allow for both CO and CO_2 production at the wall. We now compute α in Eqn. (1) using the correlation given by J.R. Arthur [8]. We call this model the Adomeit-Arthur model in reference to the fact that the data is obtained from sources [7] and [8].

All the computational details are same as in [4] and [5] and will not be repeated here. As before, we assume that the wall temperature is uniform.

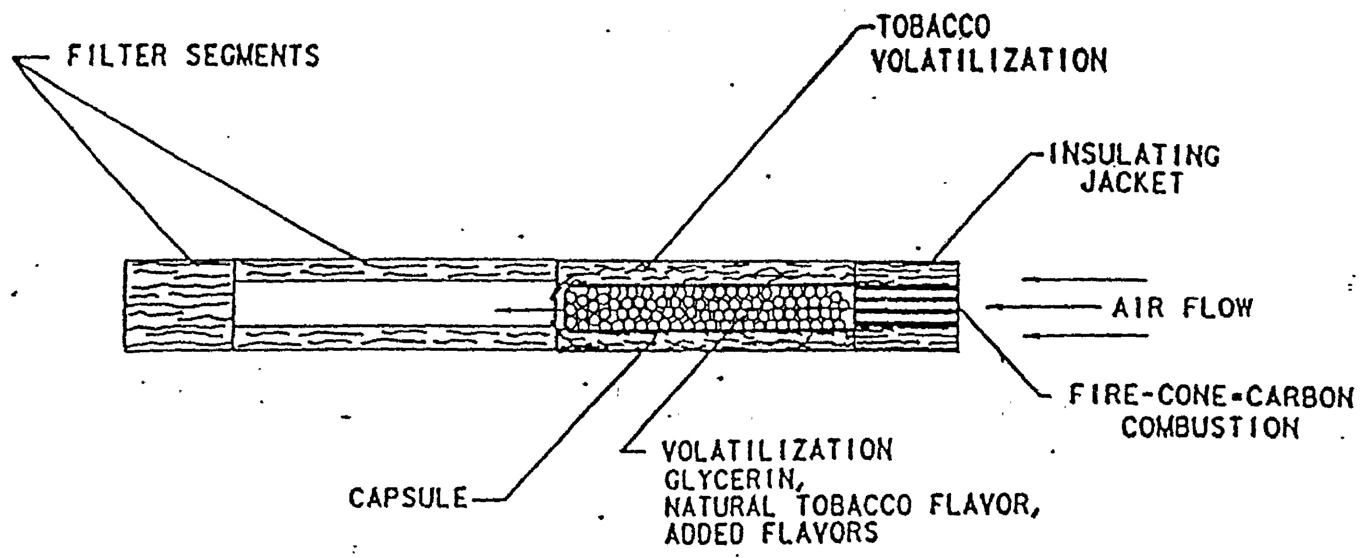

Figure 1.1: SCHEMATICS OF THE DEVICE

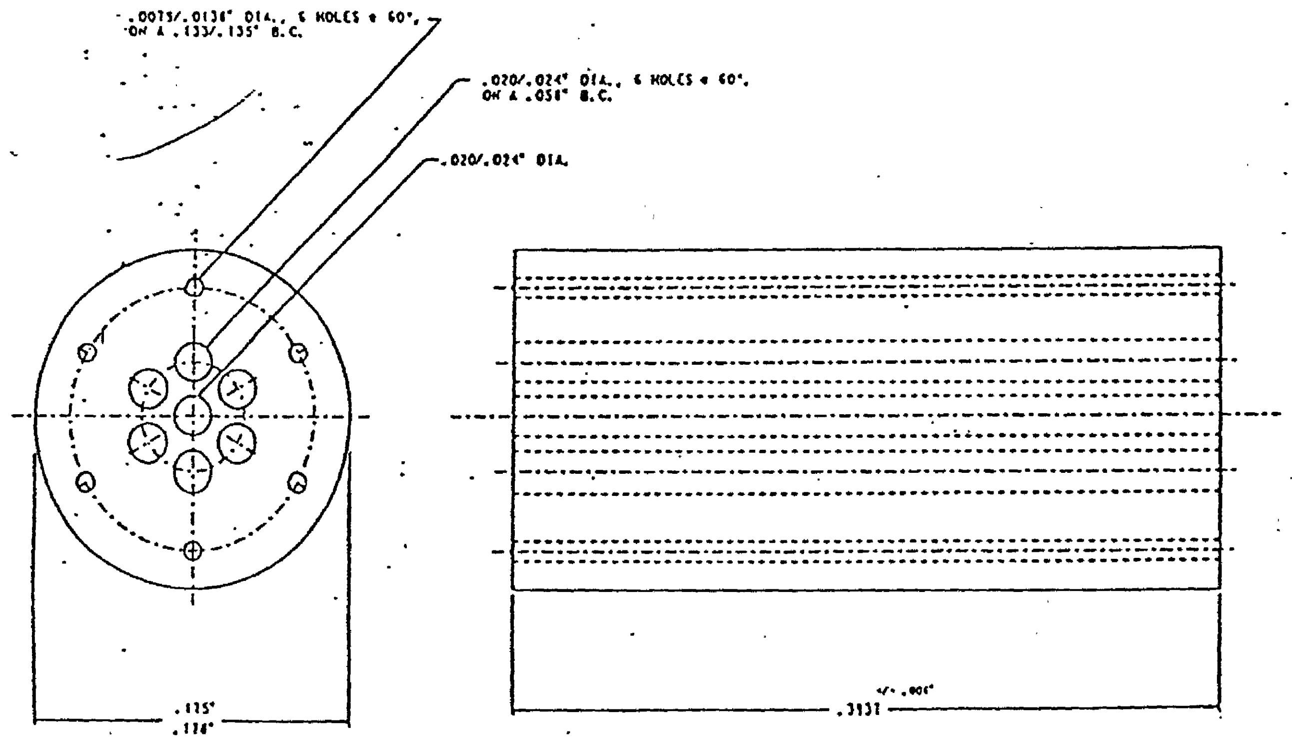

Figure 1.2: DETAILS OF THE FUEL SOURCE

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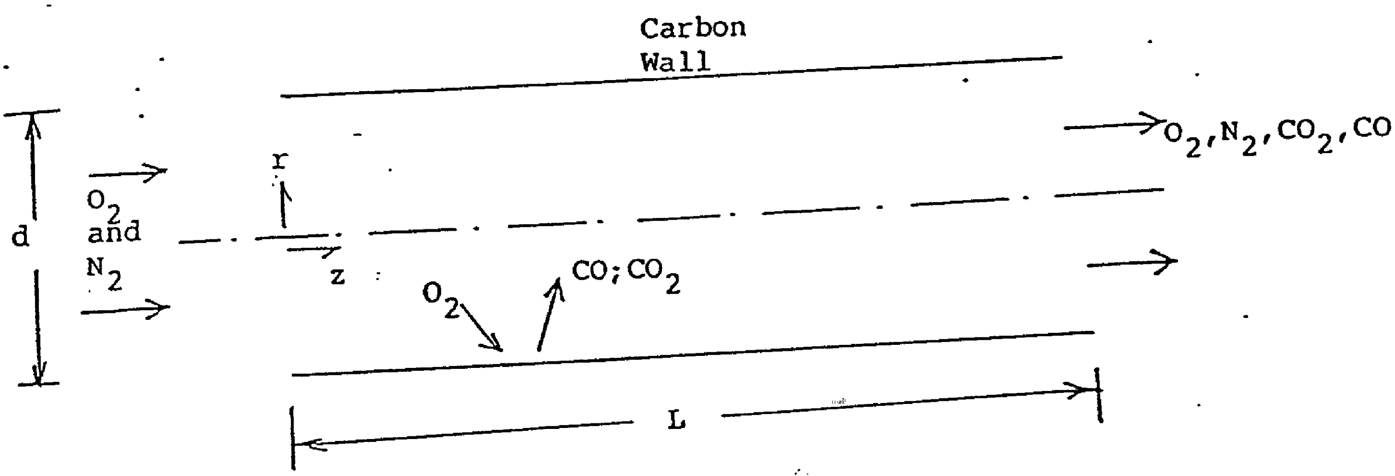

Figure 2: Schematics of Flow Through of Carbon Hole.

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2. THE ADOMEIT-ARTHUR MODEL

2.1 Results of Arthur [8]

Arthur [8] experimentally developed the following correlation for the ratio of CO to CO_2 production during hetrogenous combustion of carbon:

$$\frac{(\text{Rate of CO production})}{(\text{Rate of } CO_2 \text{ production})} = 10^{3.4} \exp\left[\frac{-E_4}{RT_w}\right] \qquad (4)$$

The above expression can be easily converted in terms of α , the fraction of C burning to CO. Thus:

$$\alpha = \frac{1}{\left\{1 + \frac{28}{44} \cdot \frac{\exp(E_4/RT_w)}{10^{3.4}}\right\}} \qquad (5)$$

It also follows that

$$\dot{m}_1 = \left\{1 + \frac{28}{44} \cdot \frac{\exp(E_4/RT_w)}{10^{3.4}}\right\} \dot{m}_{f-co} \qquad (6)$$

where

$\dot{m}_1$: total rate of carbon consumption

$\dot{m}_{f-co}$: rate of carbon consumption which results in CO production.

2.2 The Arthur-Adomeit Model

We now obtain m_{f-co} from the reaction rate data of Adomeit et.al [7], i.e.

$$\dot{m}_{f-co} = k_{0,1} \exp\left(\frac{-E_1}{RT_w}\right) \frac{\rho_w C_{O_2,w}}{W_{O_2}} \qquad (7)$$

The above expression was used in [5].

We refer to the combination of Eqns. (5), (6) and (7) as the Adomeit-Arthur model. These equations provide us the total reaction rate as well as the fraction of C burning to CO.

2.3 Constants

The constants in Eqn. (7) we presented in [5]. The only new constant we have introduced above is E_4, the activation energy in Arthur's model. The value of E_4, as given in [8], is:

$$E_4 = 12,4000 \ \frac{\text{cal}}{\text{gm-mole}} \qquad (8).$$

3. RESULTS –

The variation of α with the wall temperature is shown in Fig. 3. As discussed in [8], α increases with the temperature and, by about 1200K (1000°C), CO is practically the only product of combustion.

The variation of bulk concentration of CO and CO_2 at the exit from the hole is presented in Fig. 4. Initially the bulk concentration of CO at the exit from the hole increases with the wall temperature because more CO is produced at the wall (α increases with T_W). However, after a certain temperature, the gas phase reaction becomes active and begins to convert the CO produced at the wall to CO_2; thus, the CO concentration at the exit decreases, and the CO_2 concentration becomes greater than the CO concentration.

Finally, the mass flow rate at the exit from the hole and the total carbon burnout rate (mass exit – mass inlet) are presented in Fig. 5. The burnout rate increases with the wall temperature due to the enhanced reaction rate constant. However, above a certain temperature, the burnout rate becomes independent of the wall temperature as the reaction becomes diffusion controlled.

4. REFERENCES

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8. J.R. Arthur, "Reactions Between Carbon and Oxygen", Trans. Faraday Soc., Vol. 47, 1951, pp. 164–178.

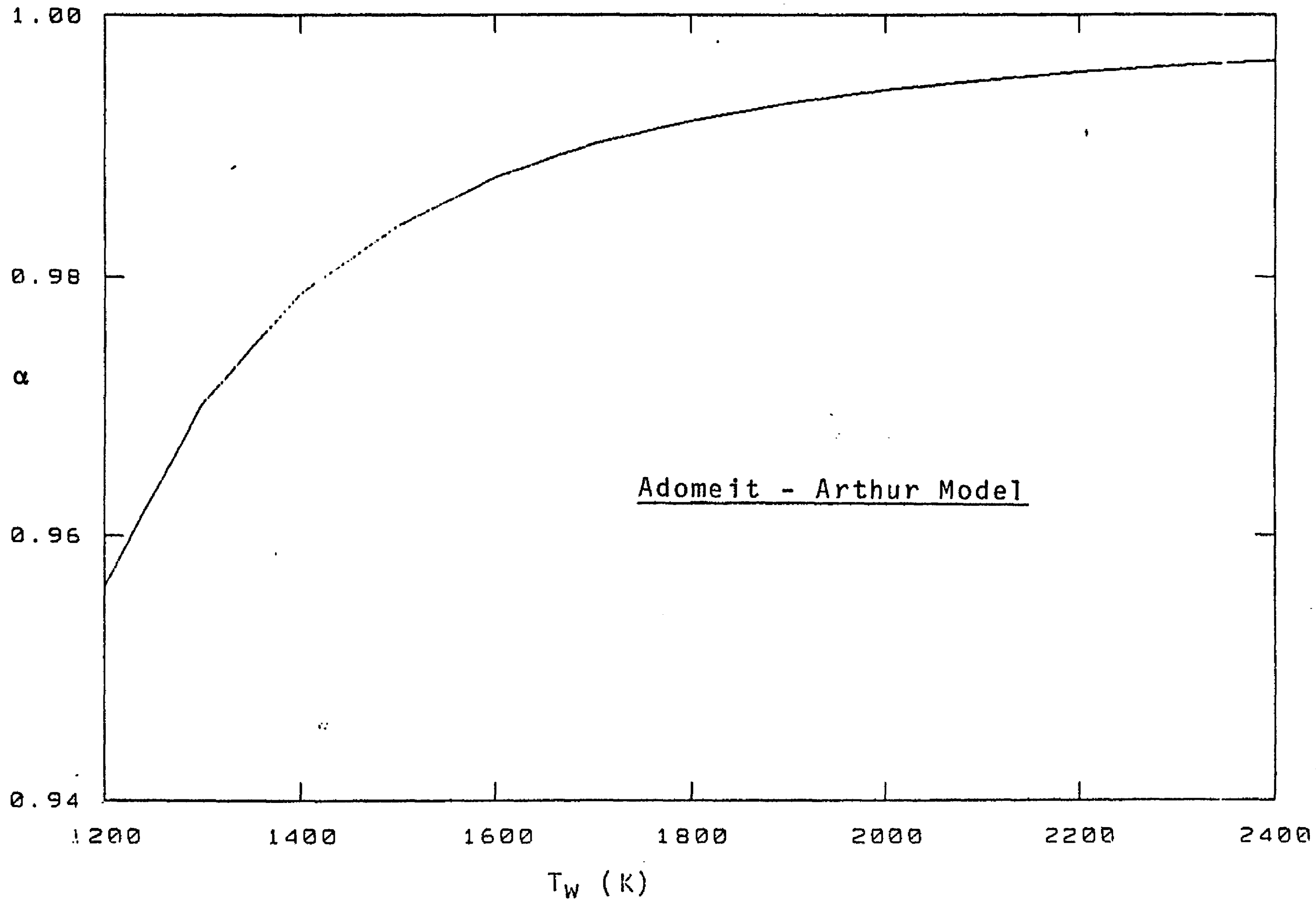

Figure 3: Variation of α

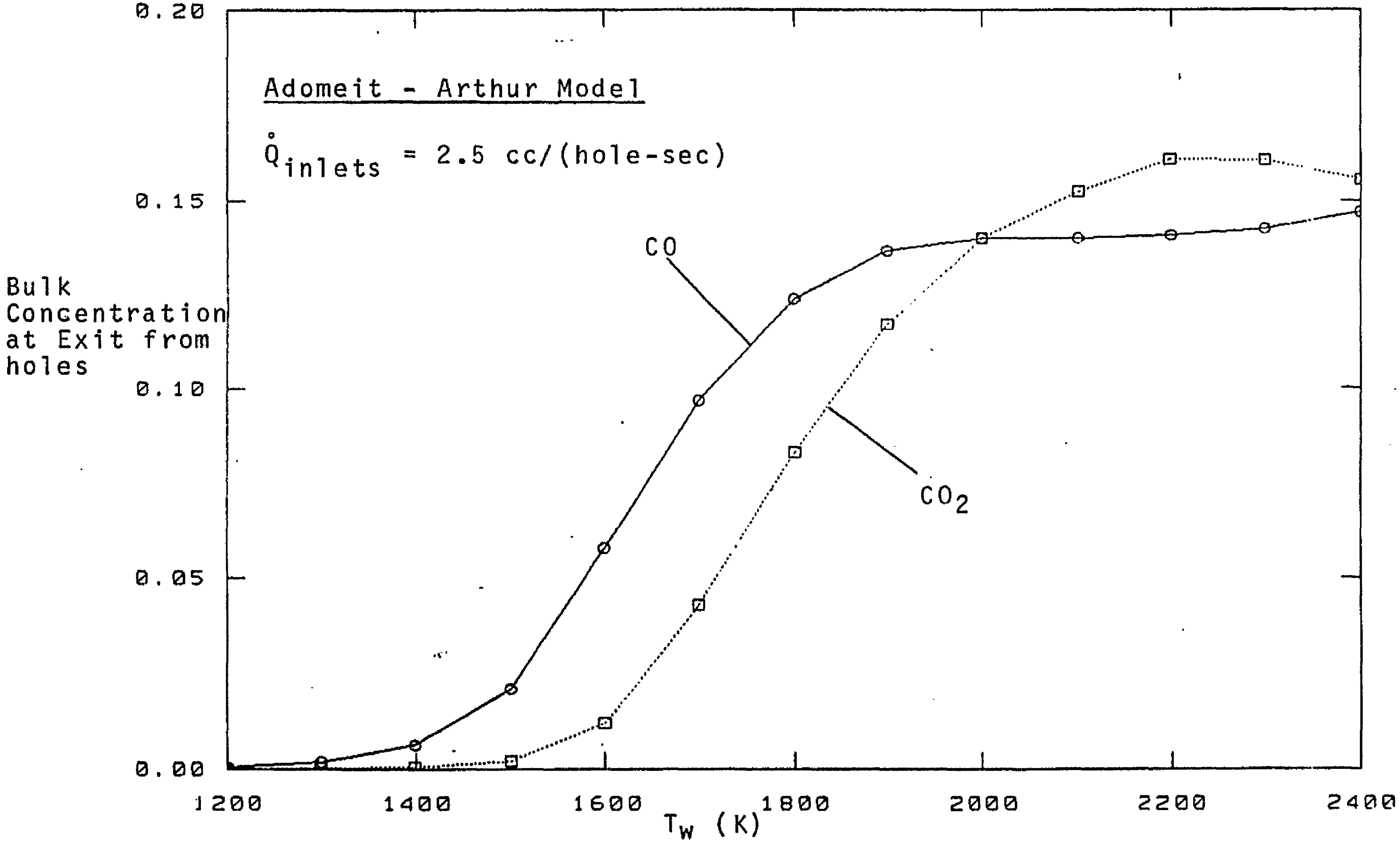

Figure 4: Variation of Bulk Concentration at Exit

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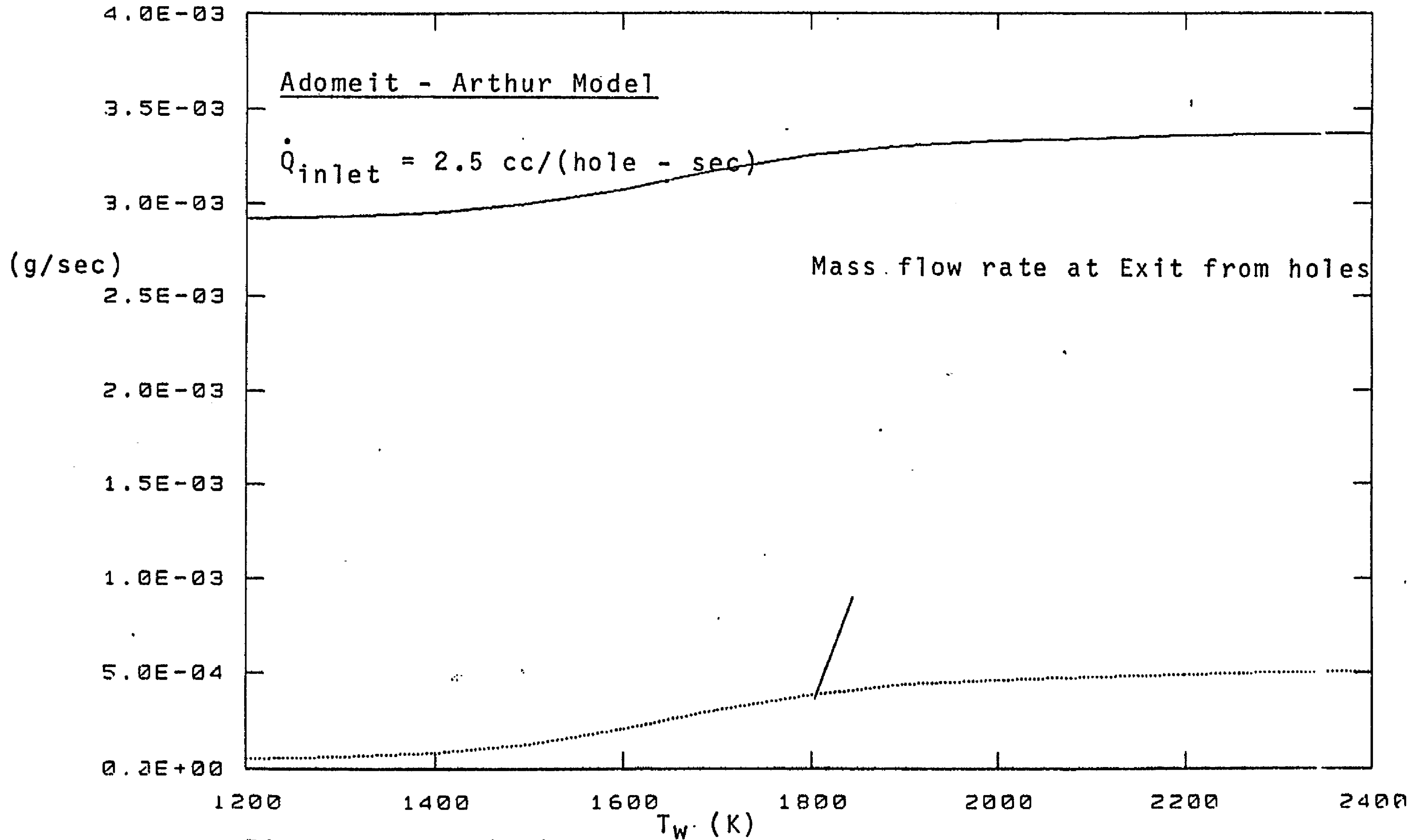

Figure 5: Variation of the total burnout rate.