

MODELING AND SIMULATION OF A FIXED-BED
REACTOR-REGENERATOR SYSTEM
FOR H₂S REMOVAL

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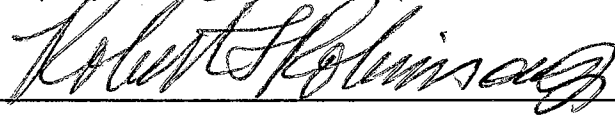
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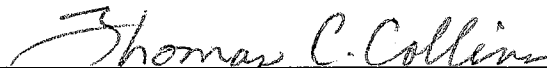


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PREFACE

A mathematical model has been developed for the description of the unsteady state behavior of an adiabatic fixed-bed reactor-regenerator system, that can efficiently remove H_2S from Claus tail gas and also increase sulfur recovery efficiency in Claus plants. In the development of this model that describes both the sulfidation and regeneration reactions, a shrinking core model and an one-dimensional heterogeneous model were used to describe the kinetics of a single sorbent and the interstitial fluid in the fixed-bed, respectively. ZnO/Al_2O_3 was used as the sulfur removal sorbent in this study.

Two dynamic simulation models (i.e., simulation programs for the sulfidation and regeneration) were developed separately in order to test the performance of the developed mathematical model.

From the sulfidation simulations for both the lab-scale system and the pilot plant scale system, the H_2S breakthrough curves have been obtained as a function of the sulfidation time. Also, the following have been predicted as a function of reactor axial position and time: H_2S gas concentration, sulfur loading of ZnO/Al_2O_3 sorbents, sorbent conversion and gas and sorbent temperatures. From the regeneration simulations for the above two systems, the O_2 breakthrough curves and the effluent SO_2 concentration profiles have been predicted as a function of the regeneration time. Also, the following have been predicted as a function of regenerator axial position and time: O_2 gas concentration, sulfur loading of ZnS/Al_2O_3 sorbents, gas and sorbent temperatures.

From parametric studies for the lab-scale system, the effects of various

parameters on the system behavior have been presented. Simulation results of the lab-scale and pilot plant scale systems were compared in terms of sorbent utilization and the temperature difference between gas and sorbent.

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NOMENCLATURE

- A gaseous reactant, H_2S or O_2
- a_{sv} interfacial area per unit volume of the fixed-bed, cm^2/cm^3
- B solid reactant, ZnO or ZnS
- $(\text{Bi})_h$ Biot number for heat transfer, dimensionless
- b stoichiometric coefficient, dimensionless
- BFW boiler feed water
- C_A molar concentration of A in the sorbent, mol/cm^3
- C_{Ab} molar concentration of A in the bulk gas stream, mol/cm^3
- C_{Abo} initial C_{Ab} , mol/cm^3
- C_{Ac} molar concentration of A at the shrinking core surface, mol/cm^3
- C_{Ao} initial molar concentration of A, mol/cm^3
- C_{As} molar concentration of A at the outer surface of the sorbent, mol/cm^3
- C_B molar concentration of B, mol/cm^3
- C_{Bo} initial molar concentration of B, mol/cm^3
- COND condenser
- C_p heat capacity (for each compound: $C_{p\text{Al}_2\text{O}_3}$, $C_{p\text{CO}_2}$, $C_{p\text{H}_2\text{O}}$, $C_{p\text{H}_2\text{S}}$, $C_{p\text{N}_2}$, $C_{p\text{O}_2}$, $C_{p\text{ZnO}}$, and $C_{p\text{ZnS}}$), $\text{cal}/\text{mol}\cdot\text{K}$ or $\text{cal}/\text{g}\cdot\text{K}$
- C_{pg} average heat capacity of feed gas, $\text{cal}/\text{g}\cdot\text{K}$
- C_{ps} average heat capacity of sorbent, $\text{cal}/\text{g}\cdot\text{K}$

- D fixed-bed diameter, cm
- D_{AB} bulk diffusivity, cm^2/h or cm^2/s
- D_c combined diffusivity from Knudsen and bulk diffusion, cm^2/h or cm^2/s
- D_e effective diffusivity of A in the product layer or within the sorbent, cm^2/h
- D_m molecular diffusivity, cm^2/h or cm^2/s
- D_K Knudsen diffusivity, cm^2/h or cm^2/s
- d sorbent diameter, cm
- d_{pe} equivalent sorbent diameter, cm
- G gaseous product, H_2O or SO_2
- g stoichiometric coefficient, dimensionless
- GHSV gas hourly space velocity, 1/h
- ΔH heat of reaction at operating temperatures ($\Delta H_{700\text{K}}$, $\Delta H_{800\text{K}}$, etc.), cal/mol
- $\Delta H_{298\text{K}}$ heat of reaction at STP, cal/mol
- h gas-solid heat transfer coefficient, $\text{cal}/\text{cm}^2\cdot\text{h}\cdot\text{K}$
- ΔH_f standard heat of formation (for each compound: $\Delta H_{f\text{H}_2\text{O}}$, $\Delta H_{f\text{H}_2\text{S}}$, $H_{f\text{O}_2}$, $\Delta H_{f\text{SO}_2}$, $\Delta H_{f\text{ZnO}}$, and $\Delta H_{f\text{ZnS}}$), cal/mol
- HP high pressure
- j_h j factor for heat transfer, dimensionless
- k thermal conductivity of feed gas (for each compound: k_{CO_2} , $k_{\text{H}_2\text{S}}$, k_{N_2} , and k_{O_2}), $\text{cal}/\text{h}\cdot\text{cm}\cdot\text{K}$ or $\text{cal}/\text{s}\cdot\text{cm}\cdot\text{K}$
- k_m gas-solid mass transfer coefficient, cm/h
- k_s reaction rate constant based on the shrinking core surface, $\text{cm}^4/\text{mol}\cdot\text{h}$
- k^* Boltzmann's constant
- L fixed-bed length, cm

- LP low pressure
- l sorbent length, cm
- M molecular weight (for each compound: M_A , M_B , M_1 , and M_2), g/mol
- MDEA methyldiethanolamine
- N_A moles of component A, mol
- Nu Nusselt number, dimensionless
- P fixed-bed operating pressure, atm
- Pr Prandtl number, dimensionless
- R sorbent radius, cm
- R_g ideal gas constant, $\text{cm}^3\cdot\text{atm}/\text{mol}\cdot\text{K}$
- r radial distance in a sorbent, cm
- r_A reaction rate of A based on unit surface of the shrinking core, $\text{mol}/\text{cm}^2\cdot\text{h}$ or $\text{mol}/\text{cm}^2\cdot\text{s}$
- r_{Av} reaction rate of A per unit volume of the fixed-bed reactor, $\text{mol}/\text{cm}^3\cdot\text{h}$ or $\text{mol}/\text{cm}^3\cdot\text{s}$
- r_{Bv} reaction rate of B per unit volume of the fixed-bed reactor, $\text{mol}/\text{cm}^3\cdot\text{h}$ or $\text{mol}/\text{cm}^3\cdot\text{s}$
- r_c shrinking core radius, cm
- r_e equivalent radius of a sorbent, cm
- r^* mean pore radius, cm
- REHTR reheater
- S solid product, ZnS or ZnO; or unit surface of the shrinking core, cm^2
- Sc Schmidt number, dimensionless
- Sh Sherwood number, dimensionless

- s stoichiometric coefficient, dimensionless
- T fixed-bed operating temperature, K
- T_g gas temperature, K
- T_g dimensionless gas temperature
- T_{g0} initial gas temperature, K
- T_s sorbent temperature, K
- T_s dimensionless sorbent temperature
- t time, s or h
- t dimensionless time
- U superficial gas velocity, cm/h
- v volumetric gas flow rate, cm³/h
- w sorbent charge, g
- WHB waste heat boiler
- wt wt% sulfur loading, %
- x fractional conversion of reactant sorbent B, dimensionless
- Y mole fraction (for each compound: Y_{CO_2} , Y_{H_2S} , Y_{N_2} , Y_{O_2}), dimensionless
- Y_1 mole fraction of compound 2 in gas mixture, dimensionless
- Y_2 mole fraction of compound 1 in gas mixture, dimensionless
- z axial distance down reactor measured from gas inlet, cm
- z dimensionless axial distance

Greek
symbols

- $\beta(x)$ function defined by Eq. (37) in Chapter IV

- σ characteristic Lennard-Jones length (for each compound: σ_A and σ_B), Angstroms
- σ_{AB} characteristic length (interaction value), Angstroms
- μ viscosity of feed gas (for each compound: μ_{CO_2} , μ_{H_2S} , μ_{N_2} , μ_{O_2} , μ_1 , μ_2), g/cm·s
- θ dummy variable
- Ω viscosity collision integral, dimensionless
- Ω_D diffusion collision integral, dimensionless
- ε voidage of the product layer, dimensionless
- ε_{AB} characteristic energy (interaction value)
- ε_p sorbent porosity, dimensionless
- ε_v voidage of the fixed-bed, dimensionless
- ε^* characteristic Lennard-Jones energy
- ρ_g gas density, g/cm³
- ρ_s solid or sorbent bulk density, g/cm³

CHAPTER I

INTRODUCTION

Hydrogen sulfide is usually produced as a by-product of petroleum refining, coal gasification, and sour natural gas processes. This gas is an extremely dangerous pollutant and, in the presence of air or water, corrosive. Recent stringent air pollution regulations on sulfur emissions have accelerated the research for better design methods to remove H_2S from many industrial gases or streams (for example, Claus tail gas, amine off-gas, coal gasifier streams, and refinery process streams).

At present, the Claus process for converting H_2S to elemental sulfur and water by the oxidation and/or the catalytic reaction from acid gas streams is used world-wide for sulfur recovery (Bell, 1992). In 1990, U.S. sulfur-recovery capacity, primarily in petroleum refineries, was at 28.5 % of the world capacity (96,916 metric tons/day) (True, 1991). These days, principal objectives of industry operating the Claus process are maximum recovery of marketable sulfur as an end product and minimum sulfur emission to the environment.

However, the total conversion (90-98%) of the Claus process is not sufficiently high (Mizuta, et al., 1991; Swain, 1991) to meet existing or future sulfur-emission environmental standards in the U.S. The incomplete conversion is due to the equilibrium relationships of the chemical reactions upon which the Claus process is based (Kohl and Riesenfeld, 1985). From studies on the theoretical equilibrium conversions of hydrogen sulfide to elemental sulfur (Figure 1) by several investigators (Gamson and Elkins, 1953;

McGregor, 1971; Bennett and Meisen, 1973; Bonsu and Meisen, 1985), the lowest possible operating temperature for Claus reactors is recommended for maximum sulfur recovery (Beshar and Meisen, 1990). A schematic representation of a typical Claus process is shown in Figure 2.

In order to reduce emission of hydrogen sulfide to the atmosphere to the level required by air pollution control authorities, the tail gases (containing about 1.0 volume % of H_2S and SO_2 (Beshar and Meisen, 1990)) from even the most efficiently designed Claus plants require further processing. Some modern Claus plants are equipped with tail gas clean-up units. These units can process the tail gases below a concentration of 200 ppm H_2S and SO_2 . For a rich acid gas feed, total sulfur recovery for the system with a tail gas treating unit approaches 99.8 % in order to meet sulfur-emission environmental standards (Swain, 1991).

Most of the known tail gas processes (for example, Sulfreen (dry-bed process); SCOT (wet-scrubbing process)) are briefly described in the following references: West, 1983; Kohl and Riesenfeld, 1985; Hydrocarbon Processing's Gas Process Handbook'90, 1990. Some of these processes are listed in Table II of literature section.

Although many different processes have been developed for the purification of Claus tail gas, no process has gained wide acceptance. The SCOT process (Figure 3) for example, is a wet-scrubbing process and is not thermally efficient because of quenching and reheating (for amine regeneration) processes. Liquid effluent from wet-scrubbing processes (other than the SCOT process) can cause waste-disposal problems. Also, the cost for tail gas clean-up must be considered as an additional cost for acid gas and this clean-up unit cost is usually too expensive. A SCOT unit may cost as much as the Claus plant (West, 1983). Sulfreen investment amounts to 40 to 55 % of the Claus unit cost for the improved version, to 30 to 45 % for the conventional version (Gas Process Handbook'90, 1990).

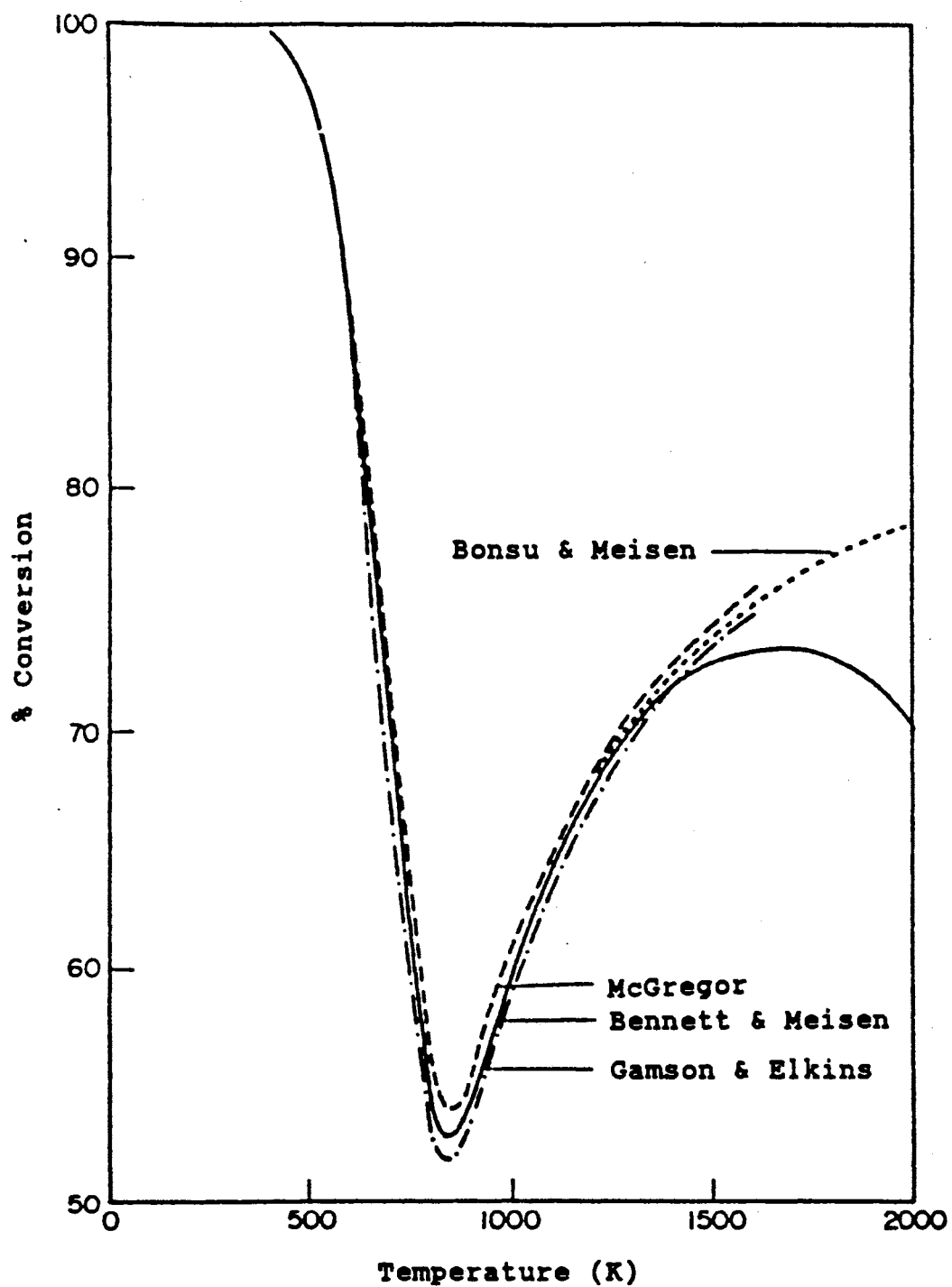


Fig. 1. Claus Reaction Equilibrium Conversion vs Temperature (Bonsu and Meisen, 1985)

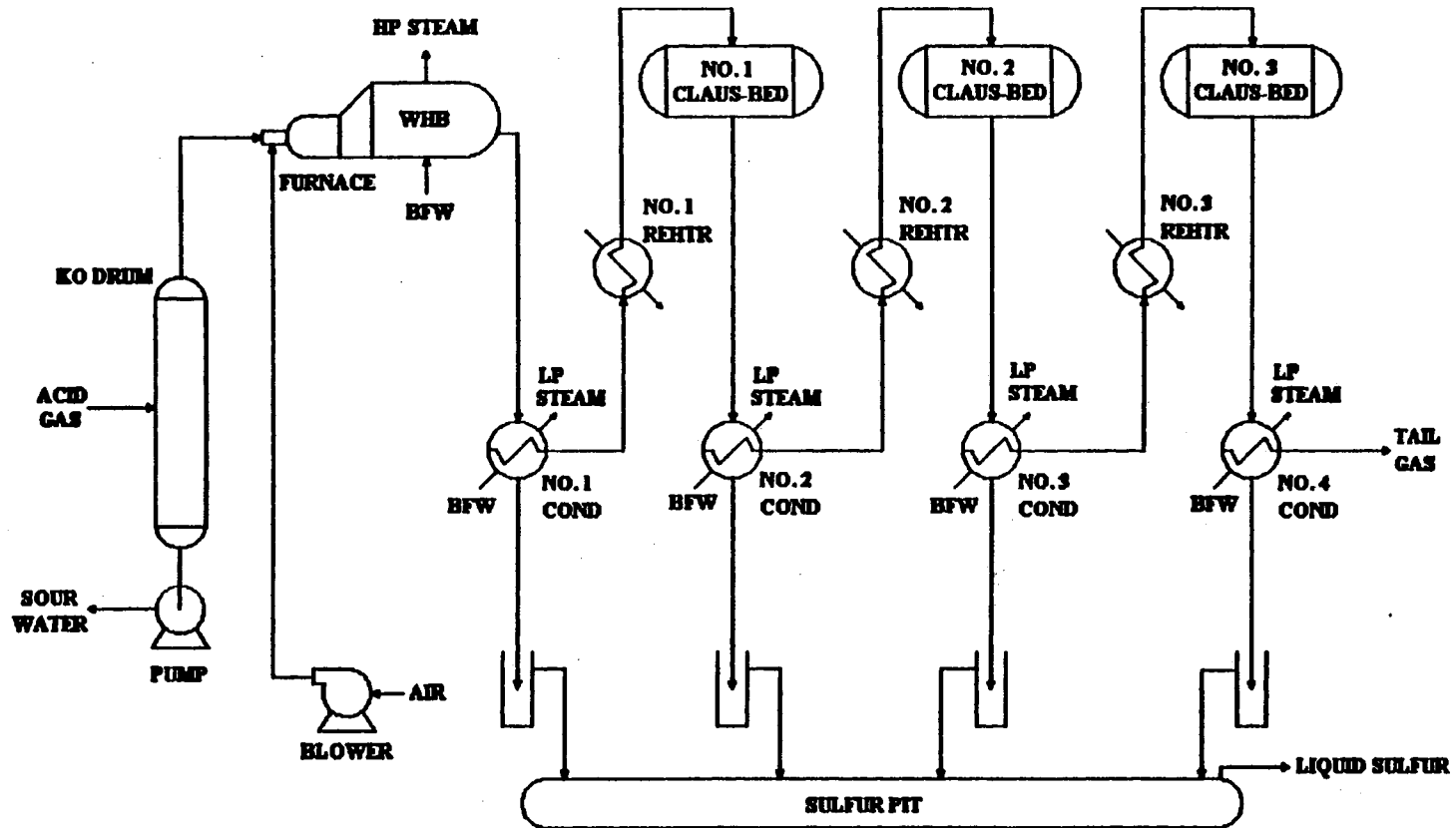


Fig. 2. Flow Diagram of Typical Claus Sulfur Recovery Process (West, 1983; Nasato et al., 1992)

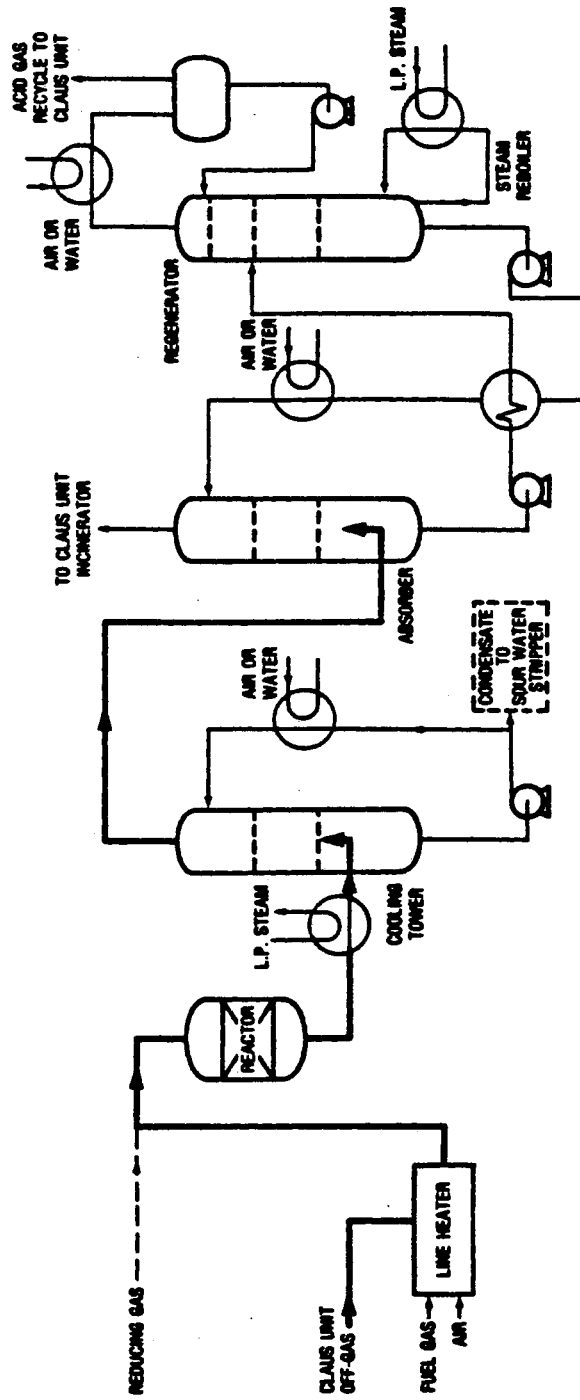


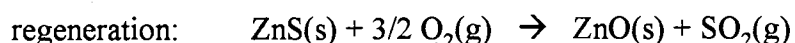
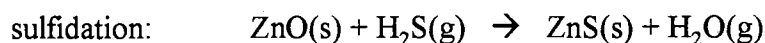
Fig. 3. Flow Diagram of SCOT Process (Kohl and Riesenfeld, 1985)

Thus, the development of an economical, thermally efficient and environmentally sound process for H₂S removal from the tail gas is a necessity. The direct removal of H₂S contained in the tail gas by using noncatalytic gas-solid reactions in a fixed-bed system may be one possible way to fulfill that necessity. However, under new stringent air-pollution regulations, this type of work hasn't been done much for the process development of Claus tail gas clean-up.

In this study, the modeling and simulation of an adiabatic fixed-bed reactor-regenerator system for H₂S removal will be done under the similar conditions to those used in commercial Claus plants. Although many new sorbents (i.e., zinc titanate, copper aluminate, zinc ferrite, etc.) have been extensively studied for high temperature coal gas desulfurization, ZnO/Al₂O₃ was selected as the H₂S removal sorbent for this work because of available R & D data from industry.

The present study has three objectives. First, a mathematical model is developed for the description of the adiabatic fixed-bed reactor-regenerator system. For this purpose, information in the following areas is required:

- (1) noncatalytic gas-solid reaction model to describe the kinetics of a single sorbent packed in the bed,
- (2) heterogeneous one-dimensional fixed-bed model for the description of the interstitial fluid,
- (3) the unsteady state nature of the sulfidation-regeneration process,
- (4) transport of heat and mass across a surface, and
- (5) the overall reactions of a sulfidation-regeneration cycle in the fixed-bed:



Second, numerical solution procedures are provided for derived governing equations of the mathematical model. FORTRAN codes are written and tested for the sulfidation and the regeneration, respectively.

Third, in order to test parameter effects on the model solutions, parametric studies are performed from the simulation results of the adiabatic fixed-bed reactor-regenerator system. In the estimation of input model parameters for the simulation, literature data and equations available and R & D data from industry are used.

From the sulfidation simulation, the following are predicted as a function of reactor axial position and time: H_2S gas concentration, sulfur loading capacity of $\text{ZnO}/\text{Al}_2\text{O}_3$ sorbents, sorbent conversion, gas temperature and sorbent temperature. The H_2S breakthrough curve is also obtained as a function of sulfidation time. From the regeneration simulation, the following are predicted as a function of regenerator axial position and time: O_2 gas concentration, sulfur loading of $\text{ZnS}/\text{Al}_2\text{O}_3$ sorbents, gas temperature and sorbent temperature. The O_2 breakthrough curve and the effluent SO_2 concentration profile are predicted as a function of regeneration time.

CHAPTER II

LITERATURE REVIEW

Modeling and simulation of a fixed-bed reactor-regenerator system for H₂S removal from Claus plant tail gases requires knowledge from many broad areas including: recent air-pollution regulations on H₂S (or SO₂) emissions, typical operating conditions of commercial Claus plants (including normal ranges of temperature, pressure and chemical composition for tail gases), various properties of presently available desulfurization sorbents (i.e., thermodynamic equilibrium, reaction rates, diffusional rates, mechanical strength), noncatalytic gas-solid reaction models, fixed-bed models, numerical solution techniques, etc.

From a preliminary literature search, the study of Claus tail gas clean-up by non-catalytic gas-solid reactions has not been reported yet, but high temperature coal gas desulfurization by non-catalytic gas-solid reactions has been extensively studied to improve power generation efficiency. Although sulfidation temperatures (600-800 K) of the tail gas clean-up system in this study are not as high as typical sulfidation temperatures (773- 973 K) of coal gas desulfurization systems, the two systems have many common general characteristics. Therefore, some of above mentioned areas are briefly described and topics (from coal gas clean-up) related with present study will be also addressed in the following sections.

Air-Pollution Regulations on H₂S (or SO₂) Emission

The Occupational Safety and Health Administration's final rules limiting H₂S as an air contaminant are as follows: TWA (Time Weight Average) is 10 ppm and STEL (Short Term Exposure limit) is 15 ppm (CFR 29, 7-1-90 edition). The Environmental Protection Agency's (EPA) final RQ (reportable quantity) of H₂S as a hazardous substance is 45.4 kg (CFR 40, 7-1-90 edition).

For refinery sulfur recovery units which process more than 20 long tons per day (LTPD) of sulfur, maximum sulfur emission rates have been set by the EPA. The principal emission limit is 250 ppmv of SO₂ discharge from the sulfur recovery plant incinerator. In order to meet the above standard, total sulfur recovery in excess of 99.8 % is required. This sulfur recovery level can only be achieved with tail gas clean-up after primary processing.

For natural gas sulfur recovery units (SRUs), proposed standards for acceptable sulfur emissions have been issued by the EPA. Table I shows mandated sulfur recovery levels as a function of total sulfur and H₂S concentration in the acid gas to be processed.

TABLE I

REQUIRED PERCENT SULFUR RECOVERY LEVELS
FROM ONSHORE NATURAL GAS SRUs
(From Pro-Quip Corp.)

Sulfur Feed Rate, LT/D	Mole % H ₂ S in Acid Gas					
	10		40		80	
	A	B	A	B	A	B
1,000	97.6	97.1	99.3	98.8	99.8	99.7
100	95.4	93.9	97.0	95.6	97.9	96.4
5	92.5	89.9	94.2	91.5	95.0	92.4
< 5	79.0	74.0	79.0	74.0	79.0	74.0

A: With fresh catalyst; B: With degraded catalyst

Developed Clean-Up Processes for Claus Tail Gas

Before strict air-pollution regulations on H₂S (or SO₂) emission were proposed, the tail gases from Claus plants were exhausted to the atmosphere through a stack without treatment or incinerated upon leaving the last Claus reactor. However, most existing Claus plants can not meet existing or proposed H₂S emission standards without addition to the original design or inclusion of a method of reducing the H₂S content of tail gases.

Some of previously developed clean-up processes for Claus tail gases are listed in Table II. Other processes such as Modop, MCRC and RSRP also have been developed. These processes are classified into two general categories: wet scrubbing processes and dry bed processes. Wet scrubbing processes use a catalytic reaction step for the conversion of sulfur compounds (other than H₂S) in the tail gas to H₂S. This H₂S is then

removed by scrubbing it with a selective solvent (for example, an aqueous MDEA solution). Dry bed processes use the same Claus reaction as that in the standard Claus process. The reaction in dry bed processes is carried below the sulfur dewpoint temperature (Kohl and Riesenfeld, 1985; Gas Process Handbook'90, 1990). These previously developed processes for tail-gas clean-up are usually expensive and frequently have waste-disposal problems.

TABLE II
DEVELOPED TAIL GAS CLEAN-UP PROCESSES
(From West (1983))

Dry-bed processes	Wet-scrubbing processes
Sulfreen Amoco cold-bed adsorption Lucas Westvaco SFGD	SCOT Beavon IFP Davy-Powergas/Wellman-Lord Cleanair ATS B & R/Selectox I Chiyoda 101 Clauspol 150

Fixed-bed Reactor-Regenerator System

In a fixed-bed reactor-regenerator system proposed for tail gas clean-up, at least two reactors are required for a pseudo-continuous operation. Thus, one unit (on-line) can be used as a sulfidation reactor and the other unit (off-line) is used as a regenerator. The fixed-bed system used in this study is shown in Figure 4. Sulfidation can be performed by passing the tail gas (or simulated H_2S -containing gas) through the bed until H_2S breakthrough occurs. Prior to breakthrough, the H_2S concentration in the desulfurized gas should be below an acceptable limit from air-quality standards. An s-shaped sulfide profile is expected in the bed at breakthrough time.

Just before (or at) breakthrough, the feed gas (i.e., tail gas) line switches to the regenerated reactor and the sulfided reactor starts regeneration. At the first cycle, the regenerated reactor (i.e., regenerator) also contains fresh sorbents. Multicycle operation is continued until regenerated sorbents have minimum H_2S removal capacity for an acceptable limit from emission standards, sulfur recovery requirements or economic reasons.

Similar fixed-bed systems have been investigated by many researchers. For example, Bissett and Strickland (1991) suggested upward gas flow in a coal gas clean-up sulfidation reactor because the sorbent generally becomes stronger as it sulfides and this type of operation places the more durable material on the bottom where crushing forces from the weight of the bed are greatest. They also stated that regeneration is conducted in the opposite direction to keep the upper part of the bed comparatively sulfur free to preserve its polishing potential. They also mention that the oxidative regeneration rate in a fixed bed depends on the rate of air addition.

Bagajewicz (1988) described the shape of the reaction front in the sulfidation reactor. The shape of the reaction front is mainly determined by specific reaction rates and diffusional rates. The outlet concentration uptake at breakthrough is directly

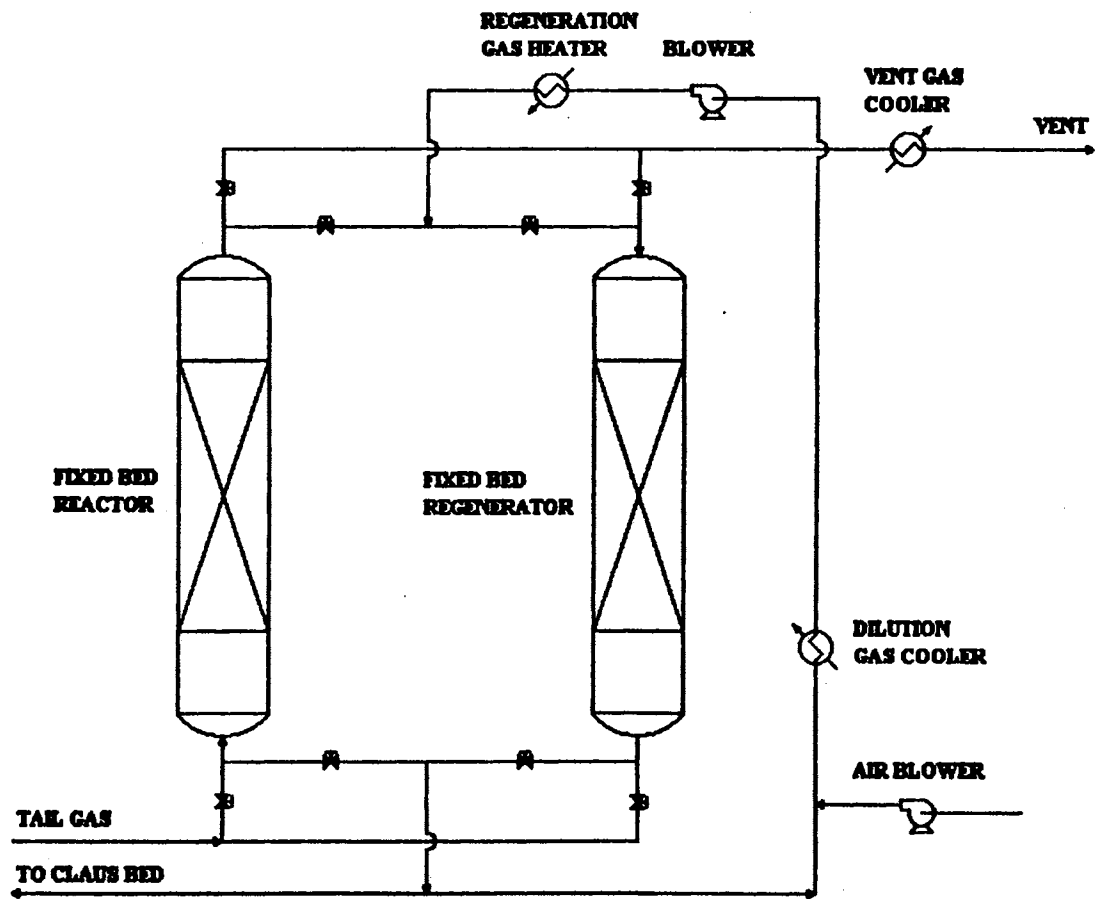


Fig. 4. Fixed-Bed Reactor-Regenerator System for Claus Tail-Gas Clean-Up

related to the shape of this front that travels along the fixed-bed reactor. Sharply decaying concentration profiles are preferred. For slowly decaying concentration profiles, the maximum acceptable level of contaminant is rapidly reached at the outlet, resulting in poor utilization of the sorbent. Thus, the width of the concentration wave is a very important parameter.

Necessary Characteristics of Sorbents for H₂S Removal

Sorbents for H₂S removal from Claus tail gases should be sufficiently reactive and regenerable with multicycle use in a fixed-bed system. Many authors have mentioned the necessary characteristics of desulfurization sorbents used for the clean-up of coal-derived fuel gas. These requirements also apply to the present study, although ZnO/Al₂O₃ sorbent does not have all of these required properties.

Sotirchos and Zarkanitis (1989) explained that hot gas desulfurization processes are based on the capacity of various metal/metal oxide solids to react with hydrogen sulfide and other sulfur-containing compounds to form metal sulfides. They also suggest that an economically feasible desulfurization sorbent should not only be regenerable but also retain its original sulfur capture capacity over multicycle testing.

Similar viewpoints for H₂S removal sorbents from other investigators (Focht, 1988; Bagazewicz, 1988; Tamhankar et al., 1986) are summarized as follows:

- 1) the degree of H₂S purification of the cleaned gas (or thermodynamic equilibrium),
- 2) sulfur loading capacity,
- 3) favorable sulfidation and regeneration kinetics,
- 4) regenerability of the sorbent,
- 5) the composition of the regeneration off-gas, and
- 6) low cost.

ZnO Sorbent for H₂S removal

Zinc oxide sorbents have been extensively studied for the efficient removal of H₂S from coal-derived gas streams at high temperatures due to the favorable thermodynamic equilibrium for ZnO sulfidation. Lew et al. (1992) and others have pointed out one possible disadvantage of these sorbents. Zinc oxide or zinc oxide containing sorbents can be partly reduced to volatile elemental zinc at temperatures above 873 K because of H₂ contained in coal gases. However, in the Claus tail gas streams, H₂ is usually not present and the zinc loss problem by reduction is not considered in this study.

Zinc oxide has been known as a thermodynamically favorable sorbent for high temperature H₂S removal and this sorbent reacts with H₂S over a wide range of pressure and temperature (Gibson and Harrison, 1980).

Westmoreland et al. (1977) studied the reaction between H₂S and ZnO over a temperature range of 573-1023 K. The initial reaction rate was measured with ZnO powder (surface area = 4.9 m²/g). The reaction was found to be first order with respect to H₂S, and the preexponential factor and activation energy were reported.

Gibson and Harrison (1980) studied the reaction between H₂S and spherical ZnO pellets (surface area = 17.9 m²/g) over a temperature range of 648-1073 K. They found rapid and essentially complete reaction in the temperature range of 873-973 K. At temperatures below 873 K, the reaction stopped well before total ZnO conversion was obtained.

Ranade and Harrison (1981) studied structural changes of ZnO sorbents due to sintering and chemical reaction. The kinetic data of Gibson and Harrison (1980) was used. Tamhankar et al. (1986) reported that the thermodynamic equilibrium for sulfidation of ZnO is quite favorable, yielding purification down to a few parts per million H₂S. The sulfidation kinetics of ZnO are much slower compared to those of iron oxide. They also

reported that the regenerability of ZnO is restricted by loss of surface area at high temperature and formation of zincsulfate at low regeneration temperatures.

Focht et al. (1988) reported that ZnO exhibits a high theoretical sulfur capacity, 393 g S per kg ZnO.

Bagajewicz (1988) found that the surface area of alumina-supported ZnO is on the order of 80-100 m²/g, which drastically increases the importance of the adsorption step. However, they concluded that adsorption can occur on ZnO as an intermediate but not as a controlling step. This adsorption also can take place on ZnS and the alumina support.

Lew et al. (1989) investigated the sulfidation performance of ZnO sorbent in a packed-bed microreactor in terms of H₂S breakthrough curves. From successive sulfidation cycles each followed by regeneration with a 10 mol % air-90 mol % N₂ at 973 K for ZnO sorbent, complete sorbent conversion and subequilibrium (below 5 ppm) H₂S levels were shown. They stated that this is in agreement with previously reported data for ZnO sulfidation (Flytzani-Stephanopoulos et al., 1985; Tamhankar et al., 1986).

Chemical Reactions of a Sulfidation-Regeneration Cycle

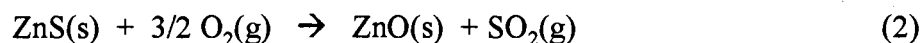
Typically, Claus tail gases contain a mixture of H₂S, CO₂, H₂O, N₂, SO₂, and traces of carbonyl sulfide. Although the relative amounts of these components depend on the type of feed acid gas and the type of sulfur recovery unit (including number of Claus stages and catalysts) used, H₂S is a major pollutant in the tail gas.

Thus, the reaction between H₂S and ZnO and the reaction between ZnS and O₂ can represent overall reactions of a sulfidation-regeneration cycle, in a fixed-bed system for tail-gas clean-up:

sulfidation:



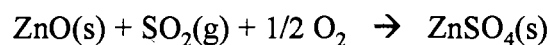
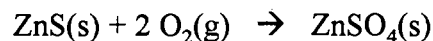
regeneration:



The sulfidation reaction (1) is exothermic and occurs very rapidly. Heat of reaction for the sulfidation reaction (1) is -14.7 kcal/mol at 700 K. ZnO is supported on alumina in order to make more ZnO accessible to the H₂S. The alumina support is not involved in chemical reactions (1) and (2). The regeneration reaction (2) is exothermic and the heat of reaction for (2) is -109.9 kcal/mol at 700 K. In the tail gas clean-up system, reaction (2) can be interpreted as follows. When sulfided sorbent (i.e., ZnS product) is regenerated, the captured sulfur is released, typically in the form of SO₂, into the regeneration gas. This SO₂ can then be recycled back to the first Claus bed where it is reacted with additional H₂S to form elemental sulfur. Thus, the role of reaction (2) is not only for the regeneration of the sulfided sorbent but also for higher sulfur recovery efficiency in Claus plants. Thus, effective integration of regeneration gas treatment into the tail gas clean-up unit is economically important in Claus plants.

Studies related with the regeneration reaction (2) are as follows. Bagajewicz (1988) performed experimental work on the regeneration of a high surface area bulk ZnO sorbent. The rate of ZnS oxidation was measured using a thermogravimetric analyzer. The kinetics of the regeneration reaction was found to follow a Langmuir-type expression over 923-973 K. Very low reaction rates were found for secondary reactions (i.e., sulfate

formations). Krishnan et al. (1985) mentioned two possible secondary reactions which can occur during the regeneration of ZnS. These side reactions are as follows:



Fukunata et al. (1976) reviewed studies on reaction (2) performed by others (Denbigh and Beveridge, 1962; Cannon and Denbigh, 1957) and pointed out discrepancies among the reported results.

Recently Developed Sorbents for H₂S Removal

Although ZnO/Al₂O₃ is selected in this modeling study, recently developed sorbents for high temperature H₂S removal will be briefly reviewed because of the possible application of these sorbents to the tail-gas clean-up system in the future.

At present, high temperature H₂S removal from coal-derived fuel gas is under intensive research, in order to meet strict environmental regulations and also improve power generation process economics. For these purposes, various supported or unsupported metal oxides (especially mixed metal oxides) have been used for sulfur sorbents.

Grindley and Steinfeld (1981) found that zinc ferrite possessed better capacity and regenerability than pure zinc oxide. Mixed ZnO-CuO has been studied for its better resistance to surface loss (Jalan, 1983), and various other mixtures including ZnO-Cr₂O₃

and ZnO-Al₂O₃ have been studied in order to increase the yield of elemental sulfur during regeneration (Anderson and Garrigan, 1982).

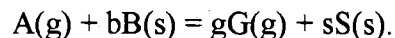
Many mixed-oxide sorbents (e.g., ZnO-Fe₂O₃, CuO-Fe₂O₃, CuO-Al₂O₃, and CuO-Fe₂O₃-Al₂O₃) were studied by Tamhankar et al. (1986) and these sorbents exhibited high H₂S removal and large sulfur capacity. More recently, zinc ferrite has been studied by investigators (Grindley, 1987; Focht et al., 1988; Focht, 1988; Gangwal et al., 1988; Focht et al., 1989; Sa et al., 1989; Bissett and Strickland, 1991; Woods et al., 1991; Ayala and Marsh, 1991).

ZnO-TiO₂ sorbents have been investigated by Flytzani-Stephanopoulos et al. (1986), Lew et al. (1989), Woods et al., (1990) and Lew et al. (1992).

Noncatalytic Gas-Solid Reactions

General Characteristics of Reactions

Gas-solid reaction means a reaction between a gas and a solid or a component of a solid. A general type of noncatalytic gas-solid reaction can be represented as



Noncatalytic gas-solid reactions involving the formation of gas and solid products (or only solid products) are an important field in chemical and metallurgical industries (e.g., the regeneration of coked catalysts, coal gasification, the reduction of metallic oxides, and the roasting and smelting of ores). A summary of various noncatalytic gas-solid reactions encountered in industry is presented in the reference by Doraiswamy and Sharma, 1984. Various aspects of these reactions are well covered by Szekely et al. (1976). Because of

recent emphasis on air-pollution control to reduce H_2S concentration from many industrial gases, noncatalytic gas-solid reactions have been extensively studied.

Such heterogeneous reactions have many similar characteristics to those of catalytic gas-solid reactions. For example, transport effects (e.g., mass and heat transfer) and reaction must be considered simultaneously. However, there is one essential difference. In noncatalytic reactions, the conditions inside the sorbent change with time because the sorbent itself is involved in the reaction. Therefore, this process is of a non-steady-state nature (Froment and Bischoff, 1990).

The steps involved in noncatalytic gas-solid reactions are similar to those in the Hougen-Watson approach for catalytic reactions (Gokarn and Doraiswamy, 1971). Wen (1968), Szekely et al. (1976), and Smith (1981) concluded that the sequence of steps in noncatalytic gas-solid reactions are:

- 1) mass transfer from bulk gas to the outer surface of the solid,
- 2) diffusion of the gaseous reactants through the porous solid or product layer,
- 3) adsorption of the gaseous reactants at the solid reactant surface,
- 4) chemical reaction between gas and solid reactants,
- 5) desorption of the gaseous products from the solid reaction surface,
- 6) diffusion of the gaseous products from the reaction surface through the porous solid or product layer, and
- 7) mass transfer from the outer surface of the solid to bulk gas.

Depending on the gas-solid reaction conditions, the step offering the highest resistance controls the overall rate. The reactions may be external mass transfer controlled, chemical reaction controlled, or pore diffusion (or product layer diffusion) controlled. The overall rate of gas-solid reaction is usually controlled by more than one step. Generally, the reacted solid retains its original geometry and dimensions. The reaction front in the solid proceeds from the outer surface to the center (Gokarn and Doraiswamy, 1971).

Types of Gas-Solid Reaction Models

Extensive studies have been reported in the literature on the models used to predict the conversion as a function of time for solids undergoing noncatalytic gas-solid reactions. Various types of models are well reviewed in several references (Doraiswamy and Sharma, 1984; Ramachandran and Doraiswamy, 1982):

Three general types of noncatalytic gas-solid reaction models (without considering structural changes) are as follows:

- 1) Shrinking core or sharp-interface model: This model is mainly applicable to a nonporous solid and the reaction is assumed to occur at a sharp interface between the exhausted outer shell and the unreacted core of the solid. The unreacted core shrinks in size as the reaction proceeds. A schematic representation of a shrinking core model is shown in Figure 5. This model will be discussed in more detail in the next section.
- 2) Homogeneous or volume reaction model: This model is used when the solid is porous and the rate of diffusion of the reactant gas is rapid. The reaction is assumed to take place all over the volume of the solid rather than at a sharp interface. A schematic of this model is shown in Figure 6.
- 3) Particle-pellet or grain model: The solid pellet is visualized as consisting of a number of small particles or grains. These particles or grains are assumed to be surrounded by macropores of the gas phase through which the gas has to diffuse to reach the various grains. The reaction occurs at the surface of each grain according to the sharp interface model. This situation is shown in Figure 7.

Noncatalytic gas-solid reaction models accounting for structural changes due to chemical reaction and/or sintering have also been developed. Some of these are modified shrinking core models, modified volume reaction models, modified particle-pellet models, single-pore models, or distributed-pore models.

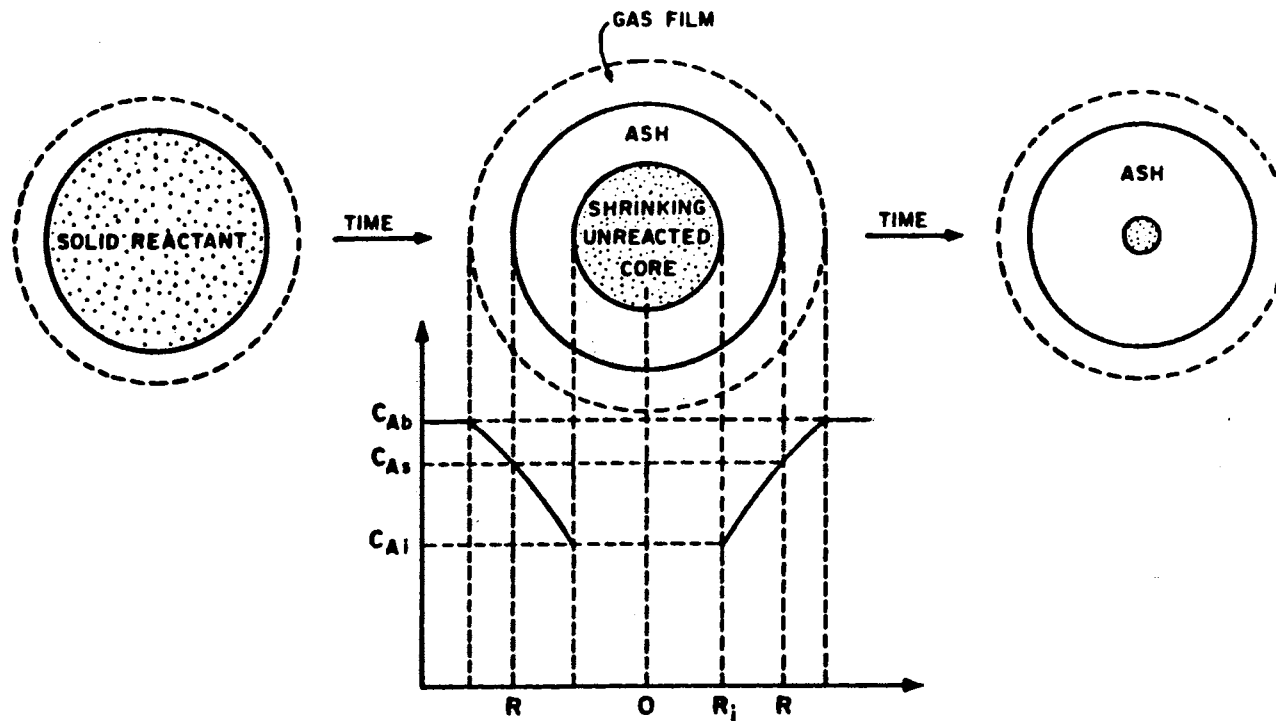
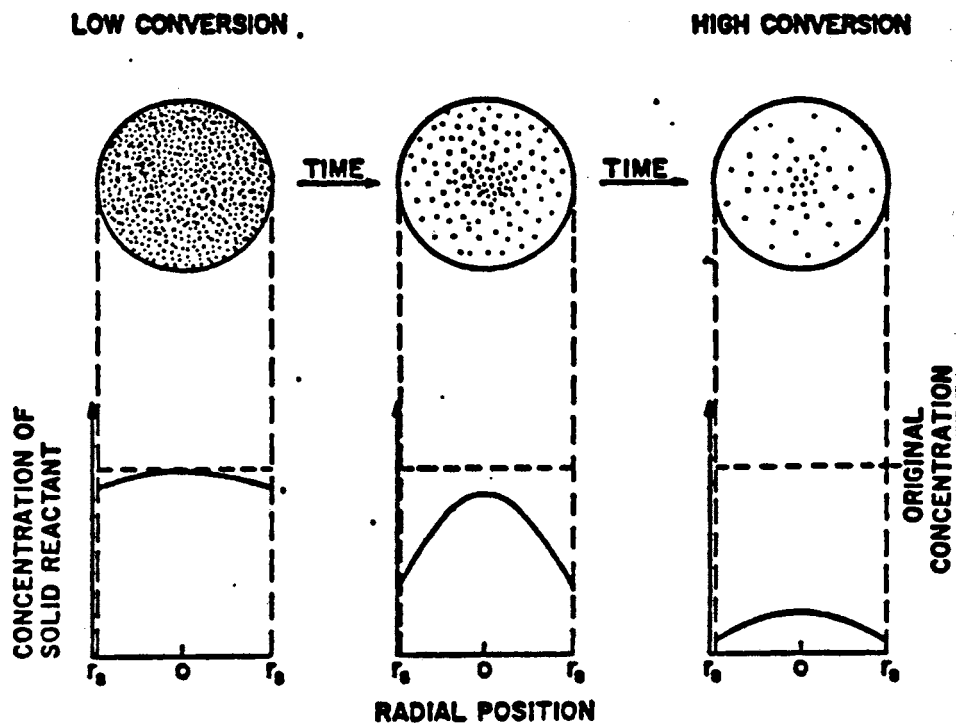


Fig. 5. Schematic of the Shrinking Core Model (Doraiswamy and Sharma, 1984)



**Fig. 6. Schematic of the Volumetric Model
(Gibson, 1977)**

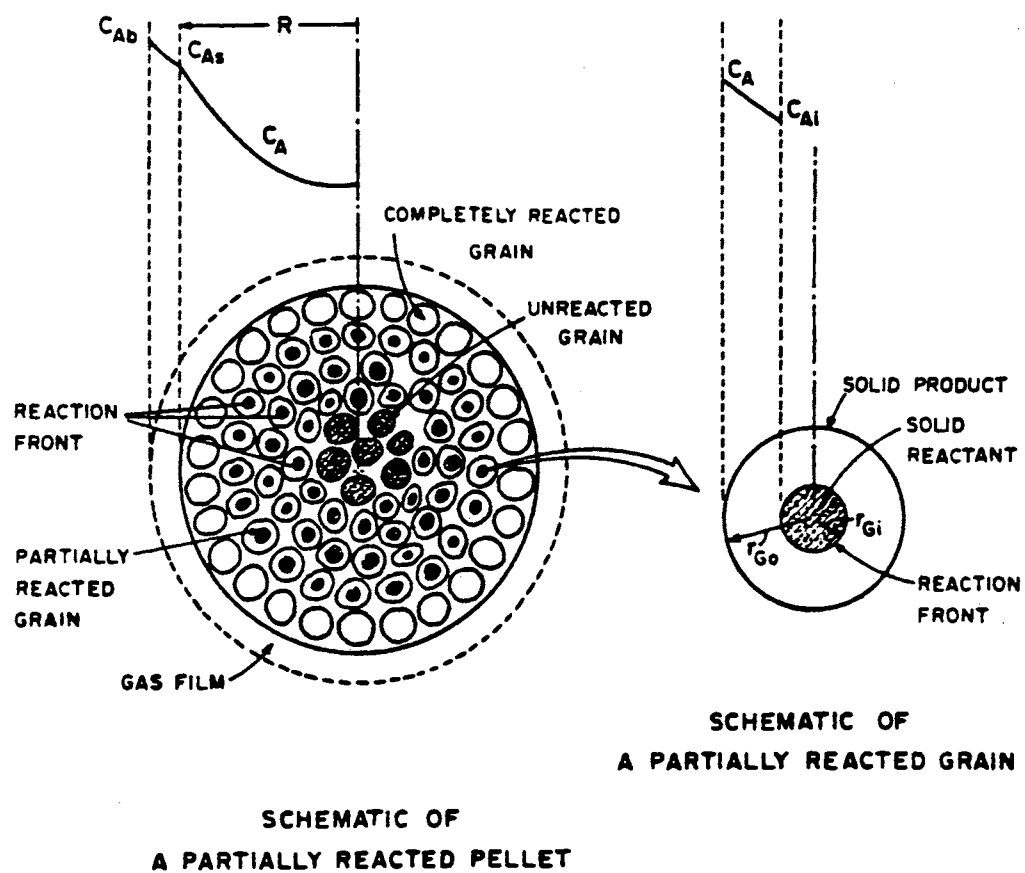


Fig. 7. Schematic of the Particle-Pellet or Grain Model (Ramachandran and Doraiswamy, 1982)

Bhatia (1991) stated that all the above models can be categorized into two groups:

- 1) Models that consider the conversion as occurring on the surface of a shrinking core with negligible internal reaction (Yagi and Kunii, 1955; Shen and Smith, 1965; Wen and Wang, 1970).
- 2) Models that consider the conversion as being dominated by internal reaction (Petersen, 1957; Szekely and Evans, 1970; Szekely et al., 1976; Ramachandran and Smith, 1977; Bhatia and Perlmutter, 1980, 1981).

Recently, general models that include both internal and external reaction have been considered by several investigators (Bhatia and Perlmutter, 1983; Chakraborty and Astarita, 1987; Bhatia, 1991a, 1991b).

Shrinking Core Model

In this tail gas clean-up study, the shrinking core model was selected to describe the kinetics of a single pellet (e.g., $\text{ZnO}/\text{Al}_2\text{O}_3$ for sulfidation and $\text{ZnS}/\text{Al}_2\text{O}_3$ for regeneration) in the fixed-bed reactor-regenerator system. Together with a fixed-bed model, the shrinking core model is used in the analysis of the transient behavior of the fixed-bed system.

Various aspects of the shrinking core model development and assumptions included in the model are briefly reviewed in this section. Governing equations for the H_2S removal sorbents in the tail gas clean-up system, based on the shrinking core model, will be derived in the model development chapter.

Yagi and Kunii (1955) first developed the shrinking core model for nonporous solid reactants. This model assumes that the reaction occurs at a sharp interface between the porous product layer and the unreacted core of the solid. They considered the rate determining step as either external mass transfer, ash diffusion, or the reaction at the

interface.

The shrinking core model is the earliest and still the most commonly used noncatalytic gas-solid reaction model because of its simplicity (Do, 1982; Bhatia, 1991). Usually, the model solution can be written in analytical form. This model is mainly applicable to highly nonporous solids and also applicable when the chemical reaction rate is very rapid and the diffusion of gases is sufficiently slow (Ishida and Wen, 1968). A sharp interface between the reactant and product may also occur in porous sorbents and the shrinking core model can be applied to those sorbents (Focht, 1988). The shrinking core model can reasonably be applied to a porous sorbent when the transport resistances (i.e., external mass transfer and internal diffusion) control the global rates (Woods et al., 1990).

In shrinking core modeling, the following assumptions are usually used:

- 1) isothermal conditions,
- 2) constant pellet (or sorbent) size,
- 3) equimolar counterdiffusion of gaseous reactants and products,
- 4) pseudo-steady-state approximation,
- 5) first order reaction, and
- 6) irreversible reaction.

Studies related with the above assumptions have been done by many investigators. The assumption of isothermal conditions is not valid for systems involving a large heat of reaction and nonisothermal models are required (Doraiswamy and Sharma, 1984). Beveridge and Goldie (1968) concluded that the pseudo-steady-state assumption generally used in the mass balance is not a good approximation for heat transfer. Thus, a transient heat balance equation including the heat capacity of the sorbent can be used in order to account for nonisothermal effects in exothermic reactions. Luss and Amundson (1969) proposed uniform and nonuniform temperature models which predict the transient temperature profiles in the pellet: the uniform temperature shrinking core model assumes

that the temperature inside each pellet is uniform at a given time. This assumption is reasonable when the thermal resistance of the pellet is very small compared to the heat transfer resistance between the gas and the pellet. The effect of thermal resistance of the pellet is considered in the nonuniform temperature shrinking core model. Prasanna et al. (1982) developed a computer program capable of predicting the transient temperature profiles in the pellet.

Models accounting for the effect of changes in pellet size due to chemical reaction have been developed by Shen and Smith (1965) for isothermal systems and by Rehmat and Saxena (1977) and Rehmat et al. (1978) for nonisothermal systems. A similar model was proposed by Mu and Perlmutter (1980). However, the pellet size change is usually not considered in shrinking core modeling.

Beveridge and Goldie (1968) analyzed the cases when the assumption of equimolar counterdiffusion results in some error. They said that the error is greatest when the diffusion in the ash layer is the main controlling step and when the transport is dominated by bulk diffusion. Gower (1971) and Sohn and Sohn (1980) also studied the effect of nonequimolar counterdiffusion (e.g., the effect of bulk flow).

Bischoff (1963), Luss (1968), and Wen (1968) studied the pseudo-steady-state approximation for gas-solid reactions. This approximation means that the rate of movement of the interface between the reactant and product is very much slower than the rate of diffusion. For this assumption, the interface can be taken to be stationary at any time and a steady state diffusion flux is used to calculate the concentration profile. They concluded that the assumption is valid when the reacting gas concentration in the bulk is much less than the molal density of the solid (e.g., $C_{Ab}M_B/\rho_B < 10^{-3}$). This approximation is satisfactory for most gas-solid systems. All the above authors studied this approximation analytically.

Sohn and Szekely (1972) studied the effect of reaction orders in noncatalytic gas-solid reactions using a shrinking core model. For the case of an n th order isothermal

reaction (e.g., for power-law kinetics), they found that the reaction order n may have a marked effect on the predictions for the rate of progress of the reaction front. They assumed that the external mass transfer was not rate controlling. Sphere and infinite slab geometries were considered.

Ramachandran (1982) analyzed Langmuir-Hinshelwood kinetics based on a shrinking core model. They found that these kinetics were a more appropriate representation than the power-law kinetics because it can represent the data over a wider range of reactant gas concentrations. The equation derived can be used to predict the conversion-time behavior of a noncatalytic gas-solid reaction following Langmuir-Hinshelwood kinetics. Chida and Tadaki (1982) analyzed four Langmuir-Hinshelwood rate expressions (i.e., nonlinear rate expressions) in terms of a shrinking core model. The effects of each expression on the gas concentration in the solid, on the effectiveness factor, and on the conversion were considered.

Examples of nonlinear, noncatalytic reactions are reported in the literature. For the oxidation of ZnS, Cannon and Denbigh (1957) reported that the reaction order was 0.5. Ong et al. (1956) and Bagajewicz (1988) suggested a Langmuir-Hinshelwood rate expression for the same reaction. However, Natesan and Philbrook (1969) and Prabhu et al. (1984) reported a first order reaction for the above reaction.

Modeling Studies for H₂S Removal In this section, H₂S removal studies with a shrinking core model describing the reaction of a single solid pellet or cylinder is briefly summarized. A summary of some significant investigations is given in Table III.

TABLE III
 H₂S REMOVAL STUDIES WITH
 A SHRINKING CORE MODEL

Authors (Year)	Reaction System (Model Type) [reaction order]	Global Rate Controlling Step(s)
Gibson (1977)	Sulfidation (Isothermal) of Zinc Oxide [first]	Internal Diffusion
Ciliberti & Lancaster (1977)	Regeneration (Nonisothermal) of Iron Sulfide [first]	External Mass Transfer & Internal Diffusion
Focht, Ranade, & Harrison (1988)	Sulfidation (Isothermal) of Zinc Ferrite [first]	External Mass Transfer & Internal Diffusion
Focht (1988)	Sulfidation (Isothermal) & Regeneration (Non-isothermal) of Zinc Ferrite [first]	External Mass Transfer & Internal Diffusion
Wang (1989)	Sulfidation (Isothermal) & Regeneration (Non-isothermal) of Zinc Ferrite [first]	External Mass Transfer & Internal Diffusion
Jothimurugesan & Harrison (1990)	Sulfidation (Isothermal) of ZnO- TiO ₂ [first]	External Mass Transfer & Internal Diffusion

Models of Fixed-Bed Noncatalytic Reactors

In this study, a fixed-bed model, together with a shrinking core model describing the reaction of single sorbents, is used in the analysis of a fixed-bed reactor-regenerator system for H₂S removal. The equations for the gas phase (i.e., mass balance and heat balance) are coupled with the equations for the reaction of a single sorbent in a fixed-bed. The system is of a transient nature because the rate of reaction decreases with time owing to the consumption of the solid reactant.

In this section, models for fixed-bed noncatalytic reactors are briefly reviewed. Three modes of contact (i.e., the fixed bed, moving bed, and fluidized bed) have been generally used for noncatalytic gas-solid reactions in industrial reactors.

Van Deemter (1953 and 1954) first studied models for fixed-bed noncatalytic reactors in order to predict the temperature distribution during catalyst regeneration by oxidation. On a much simplified model, the unsteady-state behavior of an adiabatic fixed-bed reactor was simulated and an approximate analytical solution was presented. Similar studies followed by other investigators. Johnson et al. (1962) presented an analytical solution. Van Deemter (1953, 1954) and Johnson et al. (1962) assumed temperature independence of the reaction rate. A numerical solution was developed by Gonzalez and Spencer (1963), using a second order polynomial approximation. They assumed the reaction to be temperature dependent. Olson et al. (1968) used the Runge-Kutta-Gill method to solve the system equations. The rate of movement of the combustion zone was described by a shrinking core mechanism in their model and assumed to be controlled by the diffusion. Ozawa (1969) proposed a semianalytical solution for the quasi-steady-state burning regime at lower temperatures.

However, Sampath et al. (1975) mentioned that the earlier models involve one or more limiting assumptions which cannot be adequate to describe the actual industrial practice under normal operating conditions: For example, those models did not consider

intra-pellet concentration gradients for a pellet in the reactor. Inter phase resistances to heat and mass transfer between the gas and the solid were neglected by some researchers. The transient model by Sampath et al. (1975) for fixed-bed noncatalytic reactors included the effects of inter-and intra-pellet transfer resistances and the additional effects of axial dispersion in the bulk fluid. The model was illustrated by simulating the regeneration of coked catalysts. A particle-pellet model was used for the description of the reaction of single pellets. Adiabatic and non-adiabatic operations were considered.

Marivoet and Wajc (1977) studied regeneration of a packed tubular reactor for the case of an infinitely fast gas-solid reaction. They proposed a general analytical solution and an asymptotic solution by modifying Van Deemter's model (1954).

Doraiswamy and Sharma (1984) recognized that the major contributions in the modeling of fixed-bed noncatalytic systems have been made by Evans and Song (1974), Sampath et al. (1975), and Ranade and Evans (1980). Evans and Song (1974) applied a porous pellet model to a fixed-bed reactor to predict the extent of reaction with position in a fixed-bed. Assumptions used for their fixed-bed model were as follows: plug flow of gas, isothermal behavior, uniform spherical pellets, and negligible diffusive or dispersive mass transfer in the axial direction. Mass transfer to the pellet surface from the gas stream was also assumed to be negligible.

Ranade and Evans (1980) extended the grain model to describe the reaction of a bed of solids wherein temperature and total pressure depend on position (but not time) for the nonisothermal case. Their simulation and experiments were compared using the reduction of commercial iron oxide pellets by hydrogen.

Additional studies using fixed-bed models for noncatalytic gas-solid reactions for H_2S removal are described in the next section. Other examples of studies of gas-solid reactions in fixed-bed reactors are listed in the reference by Doraiswamy and Shamma (1984).

Fixed-Bed Modeling Studies for H₂S Removal

In this section, recent fixed-bed modeling studies for H₂S removal are briefly reviewed. Different types of noncatalytic gas-solid reaction models have been studied by several investigators.

Ciliberti and Lancaster (1977) proposed a mathematical model to describe the operation of a fixed-bed reactor in which the highly exothermic regeneration of the sulfided sorbent takes place (i.e., from iron sulfide to iron oxide). Their model was used to determine an effective diffusion coefficient by correlation of computed temperature rises and reaction zone velocities, with those observed experimentally. Pressure and ambient temperature were used as input parameters for reactor model and were 1 atm and 400 K, respectively. Application of this model to commercial reactor design was discussed. They assumed that heat and mass can be convected axially but only heat can be conducted radially. The gas temperature was assumed to be the same as the bed temperature. A spherical shrinking core model was chosen for the gas-solid noncatalytic reaction. The rate controlling steps were assumed to be film diffusion and diffusion through the reacted ash.

Bagajewicz (1988) proposed a general mathematical model for an isothermal fixed-bed gas-solid reactor. Dimensional and non-dimensional equations were formulated with the following assumptions: 1) Properties in the radial direction are uniform (i.e., one-dimensional reactor model). 2) Continuity equations are written for both stationary and moving phases. 3) Reactor is isothermal. 4) The molar flux and the velocity of the gas phase is constant. 5) The reaction rate depends only on reactant and product concentrations. 6) Intraparticle diffusion is assumed to be fast. A survey of exact and approximate solutions for an isothermal fixed-bed gas-solid reactor equations was given. A traveling wave solution describing reaction fronts inside non-isothermal fixed-bed reactors was also studied (with exact and approximate solutions). In this study, numerical

solution methods and noncatalytic gas-solid reaction models were not considered.

Experimental sulfidation and regeneration of ZnO were studied in detail.

Sotirchos and Zarkanitis (1989) presented a detailed mathematical model for the description of the dynamic behavior of a fixed-bed reactor used for desulfurization of coal gas at high temperature. Structural models based on the generalized random pore and grain models were used. The developed desulfurization model was used to study the behavior of a laboratory-scale reactor packed with porous spherical ZnO pellets.

Simulation temperature and pressure were at 973 K and 1 atm, respectively. The effects of the structural model and the structural characteristics of the porous solid (internal surface area, porosity, and pore size distribution) on the breakthrough behavior of the reactor were investigated. Some assumptions used in the development of the fixed-bed model were as follows: 1) H_2S in the coal gas entering the reactor is assumed to be the primary contaminant. The other gaseous species contained in the mixture are assumed to be inert. 2) Heat effects associated with the occurrence of the desulfurization reaction are neglected because of the presence of small concentrations of gaseous reactant (H_2S) in the mixture. The fixed-bed reactor and the porous pellets are treated as isothermal. 3) Mixing in the axial direction is considered. 4) The local average conversion of the solid with the position in the reactor is involved. 5) First-order reaction is assumed. 6) The pseudo-steady-state approximation is used.

Wang, Groves, and Harrison (1990) formulated a time-dependent, isothermal, heterogeneous model for the description of high temperature desulfurization in a fixed-bed reactor. Assumptions used for the reactor model were as follows: 1) Plug flow of gas is assumed. 2) The shrinking core model is used to describe the reaction of individual pellets. 3) The sulfidation reaction is considered to be irreversible. 4) H_2S is assumed to be the only gaseous reactant. 5) Other possible reactions such as the water-gas shift are neglected. 6) The global reaction rate at high temperature is assumed to be controlled by transport rather than intrinsic reaction resistances. 7) The reactor is assumed to be

isothermal because of low H_2S concentrations and low global reaction rates. In their study, the concept of constant pattern behavior (Ruthven, 1984) was used to describe the reaction front movement after sufficient time (i.e., after time required to establish the constant pattern reaction front). For modeling analysis, the authors of this paper selected five experimental runs from the Research Triangle Institute bench-scale reactor studies and one run from the KRW process development reactor. In the experimental studies, two sorbents (i.e., ZnFe_2O_4 and ZnOTiO_2) were used. The pressure and temperature ranges studied were 1,520-1,840 kPa (15-18.2 atm) and 850-1,000 K. The authors of this paper adjusted the effective diffusivity within a single pellet in order to match the experimental H_2S breakthrough results.

CHAPTER III

PILOT PLANT STUDIES FOR H₂S REMOVAL

Pilot plant data from industry for reduction of Claus plant sulfur emissions were selected for modeling analysis of a fixed-bed sulfidation-regeneration system in this project. The model development and analysis are covered in chapter IV and VII, respectively.

The addition of the fixed-bed sulfidation-regeneration system (i.e., the tail gas clean-up system) to an existing Claus plant would convert H₂S in the tail gas to SO₂ for recycle to the Claus sulfur process, thus increasing the yield of elemental sulfur and reducing emissions. This type of processing for tail gas would be required if a typical Claus plant (including from two to four catalytic reaction stages) couldn't meet the minimum EPA sulfur recovery levels.

In pilot plant studies, adiabatic operation of two equal size fixed-bed reactors was done by running the sulfidation reaction at one isothermal temperature and running the regeneration reaction at a second isothermal temperature. One fixed-bed (on-line) was used as a sulfidation reactor and the other fixed-bed (off-line) was used as a regenerator.

Temperature ranges studied for the sulfidation reaction were 633-811 K and those for the regeneration reaction were 550-894 K. Optimum operating temperature for each reactor (for maximum H₂S removal) was reported. Operating pressure of the sulfidation reactor was 1.05 atm and that of the regeneration reactor was 1.6 atm. Pressure drop in each reactor was very low.

Inlet H_2S concentrations to the sulfidation reactor (i.e., H_2S concentrations in the effluent gas from the last stage of the Claus-bed) ranged from 0.3 to 4.0 vol%. Feed gas for a Claus sulfur recovery unit usually originates in an acid gas sweetening plant. This feed stream contains varying amounts of H_2S , CO_2 and H_2O . Also, small amounts of hydrocarbons and other impurities are usually present.

Inlet concentrations of O_2 to the regenerator were ranged from 1.0 to 4.0 vol%. Because the reaction of oxygen with the spent sorbent (i.e., $\text{ZnS}/\text{Al}_2\text{O}_3$) is highly exothermic, the oxygen is mixed with N_2 gas which reduces the concentration of O_2 in the regeneration gas and carries the heat away from the regenerator. An excess of O_2 can be used in order to ensure that the desired oxidation (i.e., the regeneration of $\text{ZnS}/\text{Al}_2\text{O}_3$) is accomplished.

Although the fresh $\text{ZnO}/\text{Al}_2\text{O}_3$ sorbent is very active for removing H_2S and the sorbent has a long life, the sulfur loading capacity of a regenerated sorbent decreased after considerable regeneration cycles.

The size of the fixed-bed reactor was 1.68m (D) x 1.95m (L). Cylindrical zinc oxide-alumina pellets were used as the sulfidation sorbents. The size of a fresh pellet was 0.318cm (d) x 0.953cm (l). Information on the fixed-bed reactor, packing and operating conditions is summarized in Table IV. Data in Table IV were obtained from a private communication with R & D Dept. of Phillips Petroleum Co. in Bartlesville, OK.

TABLE IV

PILOT PLANT EXPERIMENTAL CONDITIONS FOR
A SULFIDATION-REGENERATION SYSTEM
(from Phillips Petroleum Co.)

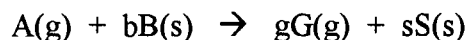
Sorbent	
type	extrudate cylinder
length(cm)	0.953
diameter(cm)	0.318
surface area(m ² /g)	50.0
mean pore radius(cm)	1.156 E-06
bulk density(g/cm ³)	1.121
Fixed-bed reactor	
bed diameter(cm)	167.6
bed length(cm)	194.8
bed voidage	0.4
sorbent charge(g)	4.815 E+06
Operating conditions	
sulfidation	
temperature(K)	633-811
pressure(atm)	1.05
inlet H ₂ S(vol%)	0.3-4.0
GHSV(1/h)	depends on operating conditions
regeneration	
temperature(K)	550-894
pressure(atm)	1.6
inlet O ₂ (vol%)	1.0-4.0
GHSV(1/h)	depends on operating conditions

CHAPTER IV

MODEL DEVELOPMENT

A mathematical model, which can be used both for an adiabatic fixed-bed sulfidation reactor and for an adiabatic fixed-bed regenerator, is developed for the efficient removal of H₂S from the Claus tail gas. In the formulation of this model, the material and energy balance equations for the sorbent and the material and energy balance equations for the fixed-bed (i.e., equations for the gas surrounding the solid sorbents in the reactor) are required. These coupled governing equations of the model account for the inter-phase heat and mass transfer resistances. The kinetics of a single cylindrical sorbent packed in the bed is described by a shrinking core model. A one-dimensional heterogeneous model is used for the description of the fixed-bed. Equations for the structural change of the sorbent during the reactions are not considered in this study.

The sulfidation model describes the sulfidation of ZnO/Al₂O₃ sorbents in an adiabatic fixed-bed reactor. The regeneration model describes the regeneration of ZnS/Al₂O₃ in an adiabatic fixed-bed regenerator. The model is developed on the basis of a noncatalytic gas-solid reaction of the following type:



The unsteady state model developed is used in the dynamic simulation of the fixed-bed system. The model parameter studies with this simulation will be useful on the design and

scale-up of a commercial scale tail gas clean-up unit. The fixed-bed reactor-regenerator system used for this study is shown in Figure 4 (Chapter II).

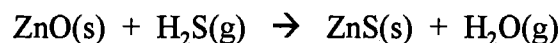
The Sulfidation Model for the Adiabatic Fixed-Bed Reactor

Details of the sulfidation model development will be presented in this section with assumptions used, governing equations for the sorbent and those for the fixed-bed.

Assumptions

The assumptions underlying the sulfidation model for the adiabatic fixed-bed reactor are summarized as follows:

1) The sulfidation reaction is first order and irreversible with respect to the gaseous reactant:



Also, the rate of this exothermic sulfidation reaction ($\Delta H_{298\text{ K}} = -14.9$ kcal/mol) is very rapid at typical operating temperatures. H_2S interaction with the alumina support is neglected.

2) H_2S is the major pollutant from a Claus-bed. The exit-gas from the Claus-bed (i.e., the last stage in a sulfur recovery unit) flows to the fixed-bed sulfidation reactor and is treated as a pseudobinary mixture of H_2S and of an inert gas (i.e., CO_2). Therefore, only one gaseous reactant (i.e., H_2S) is involved in the sulfidation reaction.

3) A shrinking core model is used to describe the reaction of a single cylindrical sorbent pellet with H_2S . From pore volume data for ZnO/Al_2O_3 used in this study ($0.27-0.29 \text{ cm}^3/\text{g}$), the model can be applied to describe reaction at the interface. The extrudates are assumed to be cylinders.

4) The rate controlling steps for the sulfidation reaction are assumed to be the external mass transfer and internal diffusion.

5) In the material balances for the sorbent and for the fixed-bed, the reactant gas accumulation terms are negligible by the pseudo steady state approximation.

6) In the energy balance for the fixed-bed reactor, the accumulation term is assumed negligible. However, in the energy balance for the sorbent, the accumulation term can not be neglected because the heat capacity of the sorbent is much greater than that of the gas.

7) Temperature gradients within a single sorbent pellet is assumed negligible.

Concentration gradients are considered within a sorbent pellet.

8) The temperature differences between the gas phase and the solid phase are considered.

9) Plug flow of gas is assumed. The effect of axial dispersion of heat and mass can be assumed negligible if the bed depth is greater than about 50 particle diameters (Carberry and Wendel, 1963). In our fixed-bed system, the ratio of bed depth to particle diameter is much greater than 50.

10) The superficial gas velocity is uniform. The pressure drop in the fixed-bed is neglected.

11) Specific heats of gas and solid, thermal conductivity, and effective diffusivity of gas are constant.

Governing Equations for the Sorbent

Derivation of governing equations for the sulfidation model begins with the description of the noncatalytic gas- solid reaction of a single solid sorbent. A shrinking core model is selected for this purpose. The energy balance equation for the sorbent will be considered in the section of the adiabatic fixed-bed system. Thus, governing equations developed from the material balance for the single sorbent will be:

- 1) the equation for the gaseous reactant concentration profile in the product layer, and
- 2) the equation for the global rate of reaction.

The Gaseous Reactant Concentration Profile in the Product layer Consider a cylindrical sorbent (uniform size during the reaction) of solid reactant B undergoing an irreversible first-order reaction with gaseous reactant A. The reaction through both ends of the sorbent is ignored. In the sorbent the molar flux of A with respect to the θ -direction and z-direction (based on the sorbent geometry) is assumed to be zero.

Under these assumptions a general model for the gas-solid reaction can be written as follows:

The equation of continuity for gaseous reactant A is

$$\frac{\partial(\varepsilon C_A)}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} \left(r D_e \frac{\partial C_A}{\partial r} \right) - r_A \quad (1)$$

Initial condition for Eq. (1) is

$$\text{at } t = 0, \quad C_A = C_{A0} \quad (2)$$

Boundary conditions for Eq. (1) are

$$\text{at } r = 0, \quad \frac{\partial C_A}{\partial r} = 0 \quad (3)$$

$$\text{at } r = R, \quad D_e \left(\frac{\partial C_A}{\partial r} \right) = k_m (C_{Ab} - C_{As}) \quad (4)$$

The equation of continuity for the solid reactant B is

$$\frac{\partial C_B}{\partial t} = -r_B = b(-r_A) \quad (5)$$

Initial condition for Eq. (5) is

$$\text{at } t = 0, \quad C_B = C_{B0} \quad (6)$$

However, for most gas-solid reaction systems, the transient term (i.e., LHS of Eq. (1)) can be neglected when

$$C_{Ab}/C_B \leq 10^{-3} \quad (7)$$

This pseudo-steady-state approximation (i.e., $\varepsilon \partial C_A / \partial t = 0$) was briefly reviewed in the literature section and is used in our sulfidation model as the condition by which Eq. (7) is satisfied.

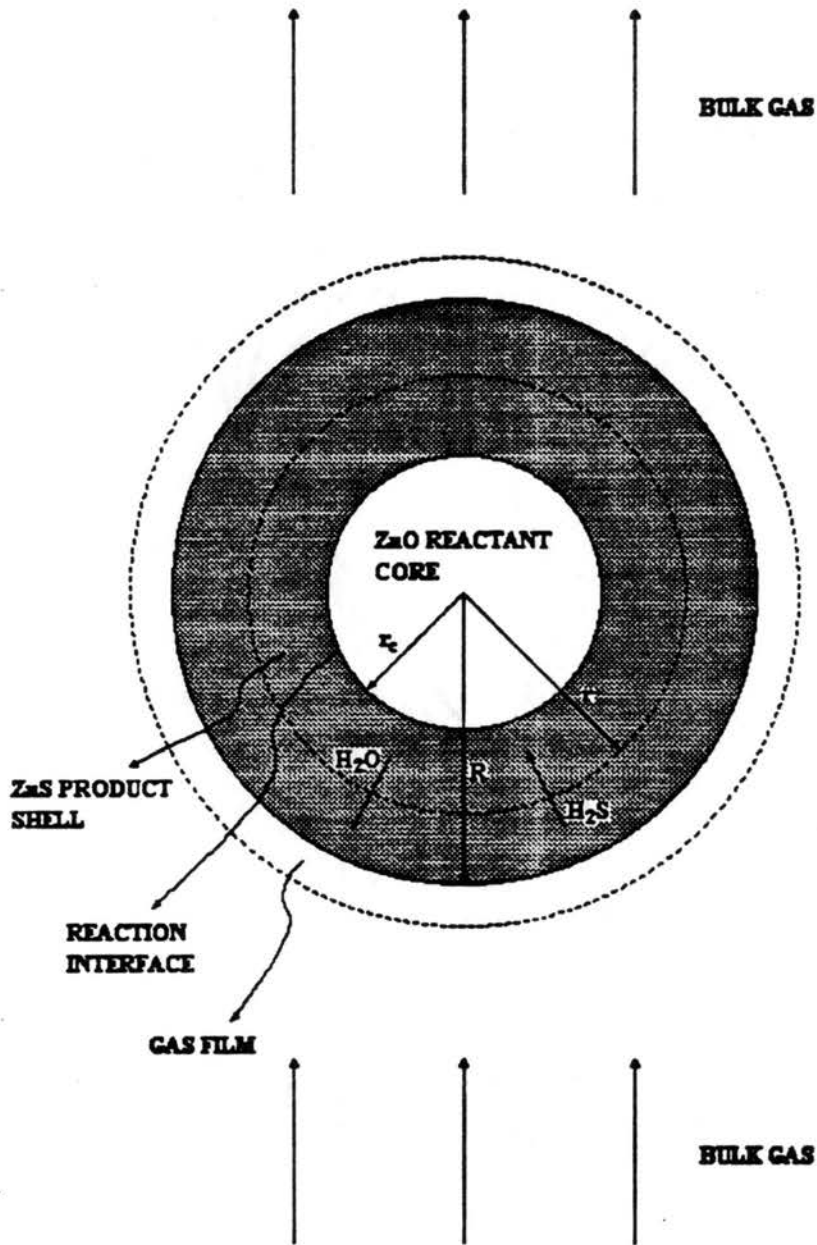


Fig. 8. Schematic of the Shrinking Core Model for the Sulfidation

Based on the pseudo-steady-state approximation and the shrinking core model as shown in Figure 8, the material balance by the general model as given in Eq. (1) becomes a material balance for the reactant component A within the product layer of the sorbent:

$$0 = \frac{1}{r} \frac{\partial}{\partial t} \left(r D_e \frac{\partial C_A}{\partial r} \right) \quad (8)$$

The boundary conditions for Eq. (8) are

$$\text{at } r = R, \quad D_e \left(\frac{\partial C_A}{\partial r} \right) = k_m (C_{Ab} - C_{As}) \quad (9)$$

$$\text{at } r = r_c, \quad D_e \left(\frac{\partial C_A}{\partial r} \right) = k_s C_{B0} C_{Ac} \quad (10)$$

In this shrinking core model, the equation of continuity for the solid reactant B and the initial condition for it are the same as those of the general model.

The symbols appearing in Figure 8 and in the above equations are designated as:

C_A is the concentration of the gaseous reactant A in the sorbent and C_{A0} is the initial concentration of A. C_{Ab} , C_{As} and C_{Ac} are the concentrations of A in the bulk of gas stream, at the outer surface of the sorbent, and at the surface of the unreacted core, respectively. C_B is the concentration of solid reactant B and C_{B0} is the initial concentration of B. D_e is the effective diffusivity of A in the product layer. The terms r , r_c and R are the radial distances from the center of the cylindrical sorbent, to any place, to the surface of shrinking core, and to the outer surface of the sorbent, respectively. k_m is

the mass transfer coefficient of A from the bulk gas phase to the sorbent surface across the film. k_s is the reaction rate constant based on the shrinking core surface. ϵ is the voidage of the porous product layer of the sorbent.

The solution of Eq. (8) with two boundary conditions, Eq. (9) and Eq. (10), gives the gaseous reactant concentration profile in the product layer:

From Eq. (8),

$$D_e \frac{\partial C_A}{\partial r} = \frac{C_1}{r} \quad (11)$$

Here, C_1 is a constant.

From two boundary conditions,

$$C_1 = Rk_m(C_{Ab} - C_{As}) = r_c k_s C_{Bo} C_{Ac} \quad (12)$$

Integrating Eq. (11) from R to r ,

$$D_e(C_A - C_{As}) = C_1 \ln \frac{r}{R} \quad (13)$$

Integrating Eq. (11) from R to r_c ,

$$D_e(C_{Ac} - C_{As}) = C_1 \ln \frac{r_c}{R} \quad (14)$$

After arranging Eqs. (12), (13) and (14), the following two equations are obtained:

$$C_{As} = C_{Ab} \frac{\frac{1}{r_c k_s C_{Bo}} + \frac{1}{D_e} \left(\ln \frac{R}{r_c} \right)}{\frac{1}{Rk_m} + \frac{1}{r_c k_s C_{Bo}} + \frac{1}{D_e} \left(\ln \frac{R}{r_c} \right)} \quad (15)$$

$$C_A = C_{Ab} \frac{Rk_m}{D_e} \ln \frac{r}{R} + C_{As} \left(1 - \frac{Rk_m}{D_e} \ln \frac{r}{R} \right) \quad (16)$$

Finally, from Eqs. (15) and (16), the gaseous reactant concentration profile in the product layer is

$$\frac{C_A}{C_{Ab}} = \frac{\frac{1}{r_c k_s C_{Bo}} + \frac{1}{D_e} \left(\ln \frac{r}{r_c} \right)}{\frac{1}{Rk_m} + \frac{1}{r_c k_s C_{Bo}} + \frac{1}{D_e} \left(\ln \frac{R}{r_c} \right)} \quad (17)$$

The Global Rate of Reaction for a Single Sorbent The rate of reaction based on unit surface of the shrinking core is

$$-r_A = -\frac{1}{S} \frac{dN_A}{dt} = \left(D_e \frac{\partial C_A}{\partial r} \right)_{r=r_c} = k_s C_{Bo} C_{Ac} \quad (18)$$

From Eqs. (17) and (18), the global rate of reaction per single sorbent is

$$\begin{aligned}
 -\frac{dN_A}{dt} &= 2\pi r_c l \left(D \frac{\partial C_A}{\partial r} \right)_{r=r_c} \\
 &= \frac{2\pi l C_{Ab}}{\frac{1}{Rk_m} + \frac{1}{r_c k_s C_{Bo}} + \frac{1}{D_e} \left(\ln \frac{R}{r_c} \right)} \quad (19)
 \end{aligned}$$

This global rate can be written in terms of sorbent fractional conversion (i.e., $x = 1 - (r_c/R)^2$):

$$-\frac{dN_A}{dt} = \frac{2\pi l C_{Ab}}{\frac{1}{Rk_m} + \frac{1}{R(1-x)^{1/2} k_s C_{Bo}} - \frac{1}{D_e} \ln(1-x)^{1/2}} \quad (20)$$

Governing Equations for the Fixed-Bed

In modeling an adiabatic fixed-bed reactor for the sulfidation reaction, the material and energy balance equations for the gas phase (i.e., equations for the fixed-bed) are coupled with the material and energy balance equations for the reaction of single sorbents. The system is of a transient nature, since the sulfidation rate decreases with time because of the consumption of the solid reactant.

Governing equations for an isothermal system are derived first and those for an adiabatic system used in this modeling study are derived next.

Isothermal Fixed-Bed System A material balance on reactant gas A and a material balance on the reactant solid B over an infinitesimal fixed-bed element as shown in

Figure 9 are required in order to describe an isothermal fixed-bed system.

The material balance on the reactant gas can be written as

$$U \frac{\partial C_{Ab}}{\partial z} + \varepsilon_v \frac{\partial C_{Ab}}{\partial t} = -k_m a_{sv} (C_{Ab} - C_{As}) \quad (21)$$

where U is the superficial gas velocity, ε_v is bed voidage, and a_{sv} is the surface area per unit volume of the bed. The transient term, $\varepsilon_v(\partial C_{Ab}/\partial t)$, is negligible compared to other terms in Eq. (21). Hence, Eq. (21) becomes

$$U \frac{\partial C_{Ab}}{\partial z} = -k_m a_{sv} (C_{Ab} - C_{As}) \quad (22)$$

The material balance on the reactant solid can be written as

$$k_m a_{sv} (C_{Ab} - C_{As}) = -\frac{(1 - \varepsilon_v)}{b} \frac{\partial C_B}{\partial t} \quad (23)$$

where b is the stoichiometric coefficient.

From Eqs. (22) and (23), the governing equation for an isothermal fixed-bed system is

$$U \frac{\partial C_{Ab}}{\partial z} = \frac{(1 - \varepsilon_v)}{b} \frac{\partial C_B}{\partial t} \quad (24)$$

where the boundary condition and the initial condition are

$$\text{at } z = 0, \quad C_{Ab} = C_{Abo} \quad (25)$$

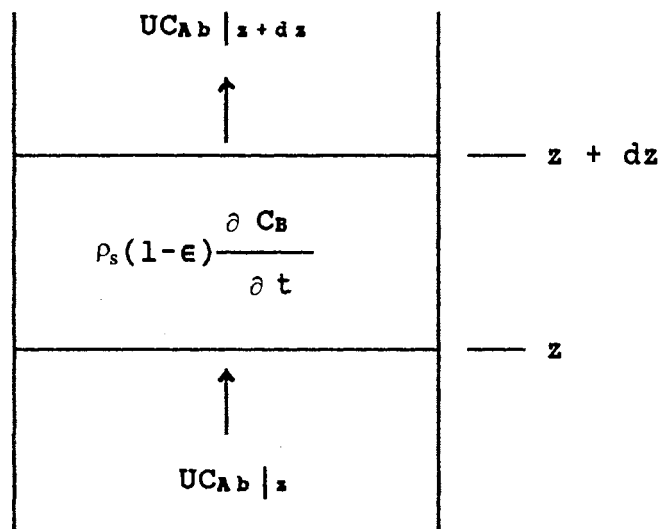


Figure 9. Schematic of the Mass Balance over a Fixed-Bed Element

$$\text{at } t = 0, \quad C_B = C_{B_0} \quad (26)$$

In Eq. (24), the solid reaction rate term (i.e., $\partial C_B/\partial t$) can be expressed as

$$-\frac{1}{C_{B_0}} \frac{\partial C_B}{\partial t} \equiv \frac{\partial x}{\partial t} \quad (27)$$

Hence, the equation (24) can be represented as

$$U \frac{\partial C_{Ab}}{\partial z} = -\frac{(1-\varepsilon_v)}{b} C_{B_0} \frac{\partial x}{\partial t} = -\frac{r_{Bv}}{b} = -r_{Av} \quad (28)$$

where r_{Av} and r_{Bv} are the rates of reaction of gas A and solid B per unit volume of the reactor.

From Eq. (20), r_{Av} can also be written as

$$r_{Av} = \frac{2(1-\varepsilon_v)}{\frac{R}{k_m} + \frac{R}{(1-x)^{1/2} k_s C_{B_0}} - \frac{R^2}{D_e} \ln(1-x)^{1/2}} C_{Ab} \quad (29)$$

Therefore, from Eqs. (28) and (29), the final dimensional governing equations for an isothermal fixed-bed system are obtained as follows:

$$\frac{\partial C_{Ab}}{\partial z} = - \frac{2(1-\epsilon_v)C_{Ab}}{U \left\{ \frac{R}{k_m} + \frac{R}{(1-x)^{1/2} k_s C_{Bo}} - \frac{R^2}{D_e} \ln(1-x)^{1/2} \right\}} \quad (30)$$

and

$$\frac{\partial x}{\partial t} = C_{Ab} \frac{2b}{C_{Bo}} \frac{1}{\left\{ \frac{R}{k_m} + \frac{R}{(1-x)^{1/2} k_s C_{Bo}} - \frac{R^2}{D_e} \ln(1-x)^{1/2} \right\}} \quad (31)$$

The boundary condition for Eq. (30) is

$$\text{at } z = 0, \quad C_{Ab} = C_{Abo} \quad (32)$$

and the initial condition for Eq. (31) is

$$\text{at } t = 0, \quad x = 0 \quad (33)$$

The above governing equations can be put into the dimensionless form:

$$\frac{\partial \bar{C}_{Ab}}{\partial z} = - \frac{\partial x}{\partial t} = - \bar{C}_{Ab} \beta(x) \quad (34)$$

with

$$\text{at } \bar{z} = 0 \text{ (for } \bar{t} \geq 0), \quad \bar{C}_{Ab} = 1 \quad (35)$$

and

$$\text{at } \bar{t} = 0 \text{ (for } \bar{z} \geq 0), \quad x = 0 \quad (36)$$

The following are used in Eq. (34):

$$\beta(x) = -\frac{2(1-\varepsilon_v)}{\frac{U}{L} \left\{ \frac{R}{k_m} + \frac{R}{(1-x)^{1/2} k_s C_{Bo}} - \frac{R^2}{D_e} \ln(1-x)^{1/2} \right\}} \quad (37)$$

$$\bar{C}_{Ab} = \frac{C_{Ab}}{C_{Abo}} \quad (38)$$

$$\bar{z} = \frac{z}{L} \quad (39)$$

$$\bar{t} = \frac{t C_{Abo} b U}{C_{Bo} L (1-\varepsilon_v)} \quad (40)$$

Eq. (34) can be written in the following integral form:

$$\frac{\partial x}{\partial t} = \beta(x) \exp \left[- \int_0^x \beta(x) d\theta \right] \quad (41)$$

where θ is a dummy variable and x is fractional conversion of reactant sorbent. Eq. (41) can be integrated by numerical procedures because $\beta(x)$ is known as a function of x (see Eq. (37)).

Adiabatic Fixed-Bed System Previously derived governing equations for the noncatalytic reaction in the isothermal fixed-bed system could be used in describing the behavior of the sulfidation system because the sulfidation reaction is not highly exothermic ($\Delta H = -14.9$ kcal/mol). However, this isothermal system is applicable only when the inlet H_2S concentration to the fixed-bed is very low.

In this sulfidation modeling project, the assumption of isothermal conditions in the fixed-bed is not likely to be acceptable because the maximum inlet H_2S concentration to the fixed-bed is as high as 4 vol%. Also, in many current Claus sulfur processes, the H_2S concentration levels in the effluent from the Claus-bed can be higher than 4 vol% and usually depends on mole % H_2S in acid gas and sulfur feed rate to the plant. Also, in industrial practice, isothermal operation of a fixed-bed noncatalytic system is not economically feasible and rarely possible because it is both expensive and difficult to remove heat at the reactor wall in order to create temperature uniformity throughout the unit. Thus, the selection of an adiabatic fixed-bed system is reasonable in the modeling of the sulfidation reaction.

The formulation of governing equations for the adiabatic fixed-bed system consists of the following balances:

- 1) material balance on the reactant gas,

- 2) material balance on the reactant solids,
- 3) energy balance on the reactant gas, and
- 4) energy balance on the reactant solids.

The same material balances for the isothermal system (i.e., Eqs. (22) and (23)) can be used as material balances for the adiabatic system. This means that the governing equations for the concentration profiles and the sorbent conversion in the fixed-bed (i.e., Eqs. (30), (31), and (34)) are used as those for the adiabatic system. Thus, energy balances on the gas and on the sorbents are only considered in this section.

On the basis of previously mentioned assumptions underlying the sulfidation model, the energy balance on the sorbents is written as

$$\begin{aligned}
 &\text{rate of heat generation due to surface reaction} - \\
 &\text{rate of heat transfer to the gas} = \\
 &\text{rate of accumulation of heat in the sorbents} \qquad \qquad \qquad (42)
 \end{aligned}$$

In the above equation, axial conduction of heat through the sorbents and radiation heat transfer effects are assumed to be negligible. However, the accumulation term can not be neglected because the heat capacity per unit volume of the sorbents is much greater than that of the gas.

Eq. (42) can be expressed mathematically based on an unit volume of the fixed-bed reactor,

$$(-\Delta H)_{Bv} - ha_{sv}(T_s - T_g) = (1 - \epsilon_v)\rho_s C_{ps} \frac{\partial T_s}{\partial t} \qquad (43)$$

After arrangement, the final energy balance on the sorbents is

$$\frac{\partial T_s}{\partial t} = \frac{(-\Delta H)}{(1-\varepsilon_v)\rho_s C_{ps}} (r_{Bv}) - \frac{ha_{sv}}{(1-\varepsilon_v)\rho_s C_{ps}} (T_s - T_g) \quad (44)$$

where r_{Bv} is, from Eqs. (28) and (29), written as

$$r_{Bv} = \frac{2b(1-\varepsilon_v)}{\frac{R}{k_m} + \frac{R}{(1-x)^{1/2} k_s C_{Bo}} - \frac{R^2}{D_e} \ln(1-x)^{1/2}} \quad (45)$$

In Eq. (44), h is the heat transfer coefficient, T_s the temperature of the sorbents, T_g the temperature of the gas, r_{Bv} the overall reaction rate of the sorbent, ρ_s the density of the sorbent, ε_v the bed voidage, C_{ps} the heat capacity of the sorbent.

The energy balance on the gas can be written as

$$\begin{aligned} &\text{rate of heat transfer to the gas} - \\ &\text{convective heat outflow} = \\ &\text{rate of accumulation of heat within the gas} \end{aligned} \quad (46)$$

Eq. (46) can be expressed mathematically based on an unit volume of the fixed-bed reactor,

$$ha_{sv} (T_s - T_g) - \rho_g UC_{pg} \frac{\partial T_g}{\partial z} = \varepsilon_v \rho_g C_{pg} \frac{\partial T_g}{\partial t} \quad (47)$$

In the above equation, the accumulation term can be neglected. Thus, the energy balance on the gas is written as

$$\rho_g UC_{pg} \frac{\partial T_g}{\partial z} = ha_{sv} (T_s - T_g) \quad (48)$$

After arrangement, the final energy balance on the gas is

$$\frac{\partial T_g}{\partial z} = \frac{ha_{sv}}{\rho_g UC_{pg}} (T_s - T_g) \quad (49)$$

where ρ_g is the density of the gas and C_{pg} is the heat capacity of the gas.

The governing equations (44) and (49) can be put in dimensionless form. From Eq. (44) with Eq. (45),

$$\begin{aligned} \frac{\partial \bar{T}_s}{\partial t} = & \frac{-\Delta H}{\rho_s C_{ps} T_{go}} \frac{2bC_{Ao}}{\frac{R}{k_m} + \frac{R}{(1-x)^{1/2} k_s C_{Bo}} - \frac{R^2}{D_e} \ln(1-x)^{1/2}} \bar{C}_{Ab} \\ & - \frac{ha_{sv}}{(1-\epsilon_v)\rho_s C_{ps}} (\bar{T}_s - \bar{T}_g) \end{aligned} \quad (50)$$

and from Eq. (49),

$$\frac{\partial \bar{T}_g}{\partial z} = \frac{ha_{sv} L}{\rho_g UC_{pg}} (\bar{T}_s - \bar{T}_g) \quad (51)$$

where $\bar{T}_g = T_g / T_{go}$ and $\bar{T}_s = T_s / T_{go}$.

In summary, the dimensional governing equations for the adiabatic fixed-bed reactor used for the sulfidation of ZnO/Al_2O_3 with H_2S are shown in Table V. Also, the dimensionless governing equations for the system are shown in Table VI.

TABLE V

DIMENSIONAL GOVERNING EQUATIONS OF THE SULFIDATION MODEL
FOR THE ADIABATIC FIXED-BED REACTOR

Material balance for the gas:

$$\frac{\partial C_{Ab}}{\partial z} = - \frac{2(1-\epsilon_v)C_{Ab}}{U \left\{ \frac{R}{k_m} + \frac{R}{(1-x)^{1/2} k_s C_{Bo}} - \frac{R^2}{D_e} \ln(1-x)^{1/2} \right\}}$$

Material balance for the sorbents:

$$\frac{\partial x}{\partial t} = C_{Ab} \frac{2b}{C_{Bo}} \frac{1}{\left\{ \frac{R}{k_m} + \frac{R}{(1-x)^{1/2} k_s C_{Bo}} - \frac{R^2}{D_e} \ln(1-x)^{1/2} \right\}}$$

Energy balance for the gas:

$$\frac{\partial T_g}{\partial z} = \frac{ha_{sv}}{\rho_g UC_{pg}} (T_s - T_g)$$

Energy balance for the sorbents:

$$\frac{\partial T_s}{\partial t} = \frac{(-\Delta H)}{(1-\epsilon_v)C_{ps}} (r_{Bv}) - \frac{ha_{sv}}{(1-\epsilon_v)\rho_s C_{ps}} (T_s - T_g)$$

where

$$r_{Bv} = - \frac{2b(1-\epsilon_v)}{\frac{R}{k_m} + \frac{R}{(1-x)^{1/2} k_s C_{Bo}} - \frac{R^2}{D_e} \ln(1-x)^{1/2}} C_{Ab}$$

TABLE VI

DIMENSIONLESS GOVERNING EQUATIONS OF THE SULFIDATION
MODEL FOR THE ADIABATIC FIXED-BED REACTOR

Material balance for the gas:

$$\frac{\partial \bar{C}_{Ab}}{\partial z} = -\bar{C}_{Ab}\beta(x)$$

Material balance for the sorbents:

$$\frac{\partial x}{\partial t} = \bar{C}_{Ab}\beta(x)$$

where

$$\beta(x) = \frac{2(1-\varepsilon_v)}{\frac{U}{L} \left\{ \frac{R}{k_m} + \frac{R}{(1-x)^{1/2} k_s C_{Bo}} - \frac{R^2}{D_e} \ln(1-x)^{1/2} \right\}}$$

Energy balance for the gas:

$$\frac{\partial \bar{T}_g}{\partial z} = \left(\frac{ha_{sv}L}{\rho_g UC_{pg}} \right) (\bar{T}_s - \bar{T}_g)$$

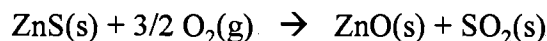
Energy balance for the sorbents:

$$\frac{\partial \bar{T}_s}{\partial t} = \frac{-\Delta H}{\rho_s C_{ps} T_{go}} \frac{2bC_{Ao}}{\frac{R}{k_m} + \frac{R}{(1-x)^{1/2} k_s C_{Bo}} - \frac{R^2}{D_e} \ln(1-x)^{1/2}} \bar{C}_{Ab} - \frac{ha_{sv}}{(1-\varepsilon_v)\rho_s C_{ps}} (\bar{T}_s - \bar{T}_g)$$

The Regeneration Model for the Adiabatic Fixed-Bed Regenerator

A mathematical model is developed for the description of the dynamic behavior of the fixed-bed regenerator used for the regeneration (i.e., the oxidation) of ZnS/Al₂O₃.

The main mechanism of the regeneration reaction is



and this reaction is highly exothermic ($\Delta H_{298\text{K}} = -109 \text{ kcal/mol}$). One gaseous reactant (i.e., O₂) is involved in the regeneration reaction and N₂ is used as a dilution gas in the fixed-bed. Possible side reactions in the regeneration process will not be considered in the modeling.

Assumptions

The assumptions underlying the regeneration model for the fixed-bed regenerator are as follows:

1) A shrinking core model (i.e., a noncatalytic gas-solid reaction model) is used to describe the reaction of a cylindrical sulfided sorbent (i.e., ZnS/Al₂O₃) with O₂.

Schematic diagram of the shrinking core model for the regeneration is shown in Figure 10.

2) The regeneration reaction is very rapid and irreversible. Several investigators have studied the reaction order of the regeneration reaction and showed discrepancies among the reported results. Cannon and Denbigh (1957) used single crystals of zinc sulfide and reported that the reaction was half-order based on experiments conducted with O₂ concentrations between 1 and 50%. Kimura et al. (1983) also reported the half-order

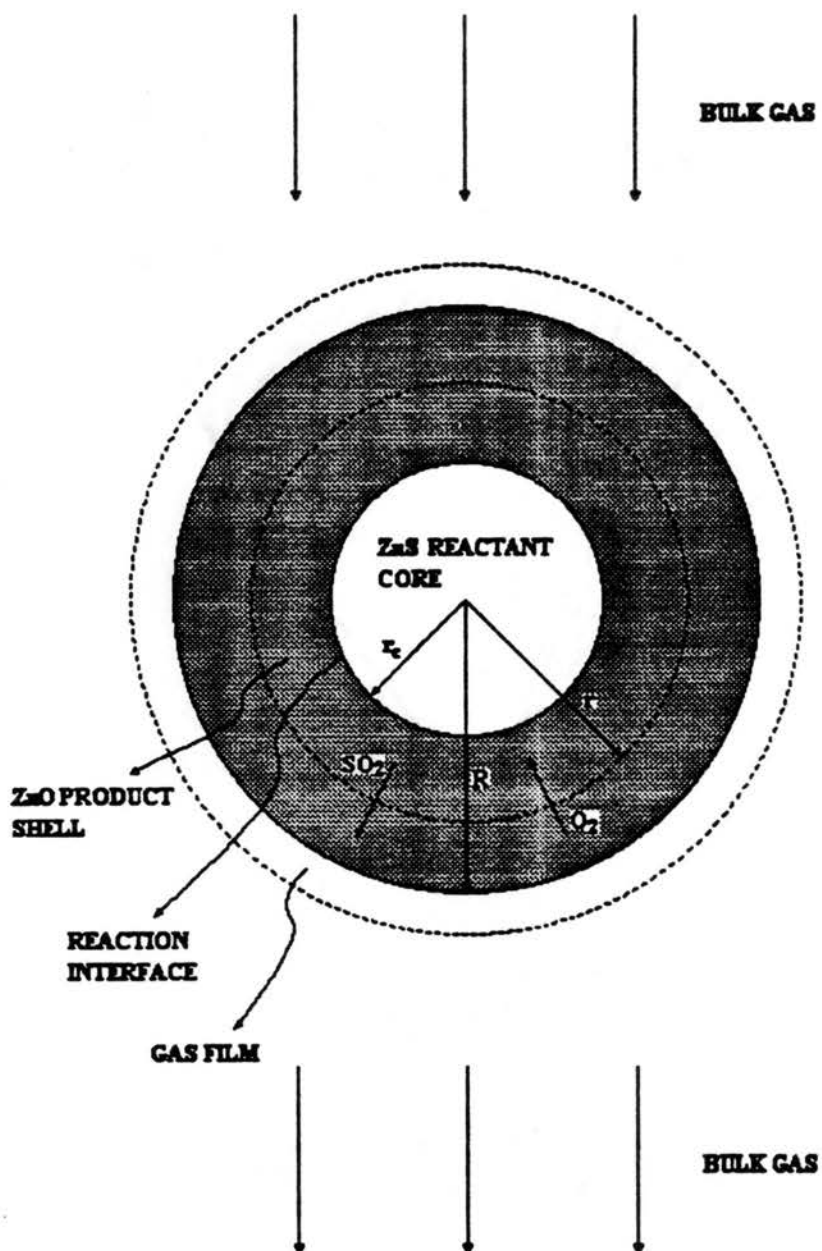


Fig. 10. Schematic of the Shrinking Core Model for the Regeneration

reaction in the same ranges of O_2 concentrations. These results are accounted for by the work of Ong et al. (1956), who also used single crystals.

However, Natesan and Philbrook (1969) and Prabhu et al. (1984) reported that the rate was first order with respect to O_2 concentration. In the study of kinetics of the oxidation of ZnS by Prabhu et al. (1984), pellet porosities of 0.724, 0.582, and 0.34 were reacted in the temperature range from 753 to 873 K. The size of cylindrical ZnS pellets were 0.95 cm in diameter and 0.7 to 1.5 cm in length. Thus, first order reaction is assumed for this study.

- 3) The rate controlling steps for the regeneration reaction are assumed to be external mass transfer and internal diffusion.
- 4) An adiabatic fixed-bed reactor is used. In the regenerator a mixture of O_2 and N_2 is passed into a thermally insulated reactor containing ZnS/ Al_2O_3 . The temperature profile will build up in accordance with the kinetics and thermodynamics of the regeneration reaction involved.
- 5) In the material balances for sulfided sorbents and for the fixed-bed, the reactant gas accumulation terms are negligible by the pseudo-steady-state approximation.
- 6) In the energy balance for the fixed-bed the accumulation term is negligible. However, in the energy balance for sulfided sorbents, the accumulation term can not be neglected because the heat capacity of sulfided sorbents is much greater than that of the gas.
- 7) Temperature gradient within a single sulfided sorbent is negligible. From experimental studies, Natesan and Philbrook (1969) and Takamura et al. (1974) reported that the temperature variation within a zinc sulfide particle undergoing reaction is extremely small.
- 8) The temperature differences between the gas phase and the solid phase are considered.
- 9) Plug flow of gas is assumed. The superficial gas velocity is assumed constant.
- 10) The pressure drop in the fixed-bed is neglected.
- 11) Specific heats of gas and solid, thermal conductivity, and effective diffusivity of gas are constant.

Governing Equations for the Regeneration Model

With the above assumptions, the derivation of the governing equations for the adiabatic fixed-bed system for the regeneration of ZnS/Al₂O₃ with O₂ showed the same governing equations as those previously derived for the adiabatic fixed-bed sulfidation model. Therefore, the governing equations shown in Table V and Table VI are also used for the regeneration model.

CHAPTER V

NUMERICAL IMPLEMENTATION

The dimensionless governing equations (shown in Table VI) of the mathematical model developed for the description of the adiabatic fixed-bed reactor-regenerator system can be considered as ordinary differential equations along the time and the dimensionless length lines as shown in Figure 11. These equations are of the following form:

$$\left(\frac{d\bar{C}_{Ab}}{dz} \right)_t = f_1(\bar{C}_{Ab}, x) \quad (1)$$

$$\left(\frac{d\bar{T}_g}{dz} \right)_t = f_2(\bar{T}_g, \bar{T}_s) \quad (2)$$

$$\left(\frac{dx}{dt} \right)_z = f_3(\bar{C}_{Ab}, x) \quad (3)$$

$$\left(\frac{d\bar{T}_s}{dt} \right)_z = f_4(\bar{C}_{Ab}, x, \bar{T}_g, \bar{T}_s) \quad (4)$$

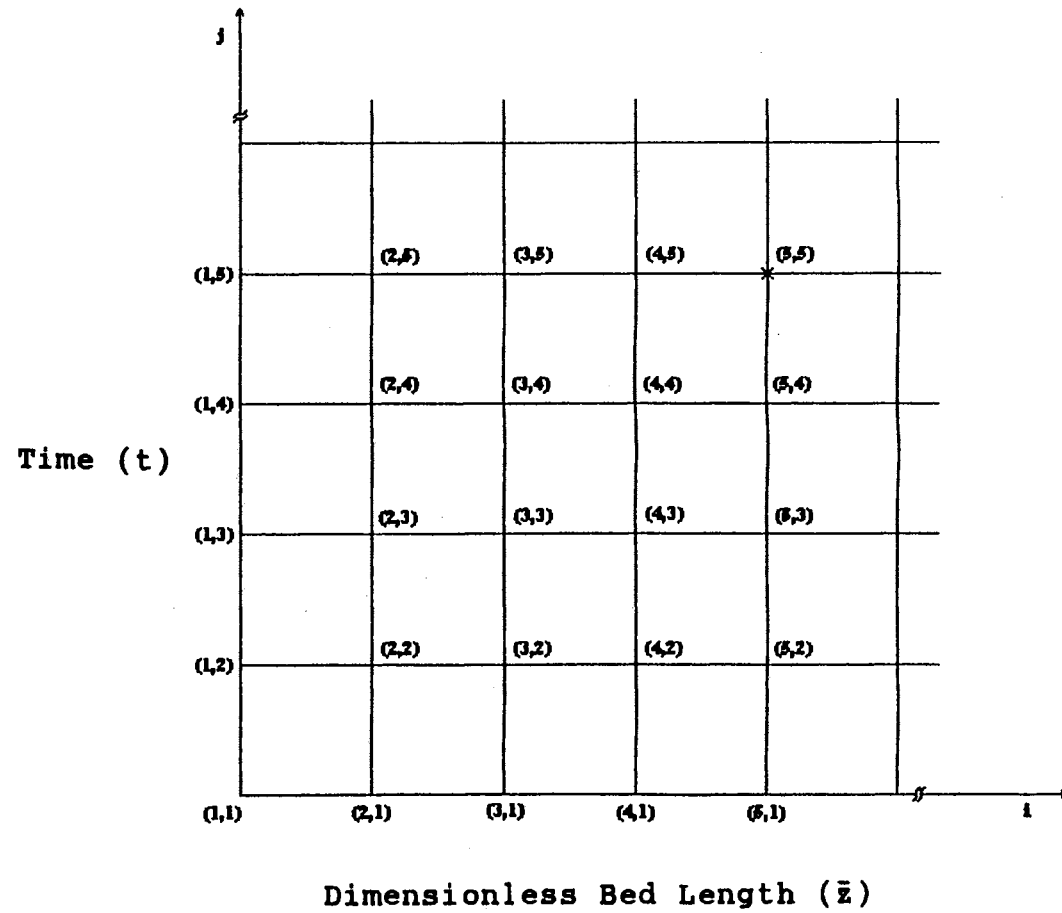


Fig. 11. Schematic of the grid lines for Integration

The above equations must be solved with following conditions :

$$\text{at } \bar{z} = 0, \quad \bar{C}_{Ab} = 1, \quad \bar{T}_g = 1 \quad (\text{for } t \geq 0) \quad (5)$$

$$\text{at } t = 0, \quad x = 0, \quad \bar{T}_s = 1 \quad (\text{for } 1 \geq \bar{z} \geq 0) \quad (6)$$

The numerical technique employed to solve these coupled ordinary differential equations consists of predictor-corrector solutions of the concentration equation, the temperature equations, and the conversion equation. A fourth-order Adams-Moulton method is used for the integration of the four equations. The predictor-corrector formulas used in this method are as follows:

Predictor:

$$Y_{n+1} = Y_n + (H/24)(55F_n - 59F_{n-1} + 37F_{n-2} - 9F_{n-3})$$

Corrector

$$Y_{n+1} = Y_n + (H/24)(9F_{n+1} + 19F_n - 5F_{n-1} + F_{n-2})$$

Here, Y is a dependant variable (i.e., \bar{C}_{Ab} , \bar{T}_g , x, or \bar{T}_s).

H represents a step size of the integration (i.e., time step or dimensionless length step). F can be an any function (i.e., f_1 , f_2 , f_3 , or f_4). The previous four grid points are represented by n, n-1, n-2, n-3 (when one characteristic line is fixed). In the corrector equation the value of F_{n+1} is evaluated with the value obtained for Y_{n+1} from the predictor equation. This means the corrector equation is implicitly calculated.

The predictor-corrector calculations are illustrated for the point $(i,j) = (5,5)$ in Figure 11, and others are obtained similarly. From the predictor equation:

$$\begin{aligned} \bar{C}_{Ab}(5,5)_p &= \bar{C}_{Ab}(4,5) + (\Delta z / 24) \left[55f_1(x(4,5), \bar{C}_{Ab}(4,5)) - 59f_1(x(3,5), \bar{C}_{Ab}(3,5)) \right. \\ &\quad \left. + 37f_1(x(2,5), \bar{C}_{Ab}(2,5)) - 9f_1(x(1,5), \bar{C}_{Ab}(1,5)) \right] \end{aligned}$$

$$\begin{aligned} \bar{T}_g(5,5)_p &= \bar{T}_g(4,5) + (\Delta z / 24) \left[55f_2(\bar{T}_s(4,5), \bar{T}_g(4,5)) - 59f_2(\bar{T}_s(3,5), \bar{T}_g(3,5)) \right. \\ &\quad \left. + 37f_2(\bar{T}_s(2,5), \bar{T}_g(2,5)) - 9f_2(\bar{T}_s(1,5), \bar{T}_g(1,5)) \right] \end{aligned}$$

$$\begin{aligned} x(5,5)_p &= x(5,4) + (\Delta t / 24) \left[55f_3(x(5,4), \bar{C}_{Ab}(5,4)) - 59f_3(x(5,3), \bar{C}_{Ab}(5,3)) \right. \\ &\quad \left. + 37f_3(x(5,2), \bar{C}_{Ab}(5,2)) - 9f_3(x(5,1), \bar{C}_{Ab}(5,1)) \right] \end{aligned}$$

$$\begin{aligned} \bar{T}_s(5,5)_p &= \bar{T}_s(5,4) + (\Delta t / 24) \left[55f_4(\bar{T}_s(5,4), \bar{T}_g(5,4), x(5,4), C_{Ab}(5,4)) \right. \\ &\quad - 59f_4(\bar{T}_s(5,3), \bar{T}_g(5,3), x(5,3), C_{Ab}(5,3)) \\ &\quad + 37f_4(\bar{T}_s(5,2), \bar{T}_g(5,2), x(5,2), C_{Ab}(5,2)) \\ &\quad \left. - 9f_4(\bar{T}_s(5,1), \bar{T}_g(5,1), x(5,1), C_{Ab}(5,1)) \right] \end{aligned}$$

From the corrector equation:

$$\begin{aligned} \bar{C}_{Ab}(5,5)_c &= \bar{C}_{Ab}(4,5) + (\Delta z / 24) \left[9f_1(x(5,5)_p, \bar{C}_{Ab}(5,5)_p) + 19f_1(x(4,5), \bar{C}_{Ab}(4,5)) \right. \\ &\quad \left. - 5f_1(x(3,5), \bar{C}_{Ab}(3,5)) + f_1(x(2,5), \bar{C}_{Ab}(2,5)) \right] \end{aligned}$$

$$\begin{aligned} \bar{T}_g(5,5)_c = \bar{T}_g(4,5) + (\Delta z / 24) & \left[9f_2(\bar{T}_s(5,5)_p, \bar{T}_g(5,5)_p) + 19f_2(\bar{T}_s(4,5), \bar{T}_g(4,5)) \right. \\ & \left. - 5f_2(\bar{T}_s(3,5), \bar{T}_g(3,5)) + f_2(\bar{T}_s(2,5), \bar{T}_g(2,5)) \right] \end{aligned}$$

$$\begin{aligned} x(5,5)_c = x(5,4) + (\Delta t / 24) & \left[9f_3(x(5,5)_p, \bar{C}_{Ab}(5,5)_c) + 19f_3(x(5,4), \bar{C}_{Ab}(5,4)) \right. \\ & \left. - 5f_3(x(5,3), \bar{C}_{Ab}(5,3)) + f_3(x(5,2), \bar{C}_{Ab}(5,2)) \right] \end{aligned}$$

$$\begin{aligned} \bar{T}_s(5,5)_c = \bar{T}_s(5,4) + (\Delta t / 24) & \left[9f_4(\bar{T}_s(5,5)_p, \bar{T}_g(5,5)_c, x(5,5)_p, \bar{C}_{Ab}(5,5)_c) \right. \\ & + 19f_4(\bar{T}_s(5,4), \bar{T}_g(5,4), x(5,4), \bar{C}_{Ab}(5,4)) \\ & - 5f_4(\bar{T}_s(5,3), \bar{T}_g(5,3), x(5,3), \bar{C}_{Ab}(5,3)) \\ & \left. + f_4(\bar{T}_s(5,2), \bar{T}_g(5,2), x(5,2), \bar{C}_{Ab}(5,2)) \right] \end{aligned}$$

The iterations on the above formulas are continued until the desired accuracy is obtained. In the time-dimensionless length grids shown in Figure 11, any of the dependant variables at (i,j) can be obtained if the previous four values are known (i.e., at (i-1,j), (i-2,j), (i-3), (i-4) or at (i,j-1), (i,j-2), (i,j-3), (i,j-4)).

In this study, the values of all the dependant variables are computed along the time line, and then the time increment is increased for new profiles (at next time step): For example, at $t = 0$, Eqs. (1) and (2) are integrated from $z = 0$ to $z = 1$. The values of x and T_s are given by condition (6). With these values of four dependant variables along $t = 0$ line, a time step is increased and the predictor-corrector formulas are again applied to the dependant variables. This procedure is repeatedly used in the all grid points in Figure 11. For starting the solutions by the Adams-Moulton method, Euler's method and a simple set of predictor-corrector formulas are applied.

CHAPTER VI

MODEL PARAMETERS

In order to study the behavior of an adiabatic fixed-bed sulfidation-regeneration system, numerical values of all the parameters appearing in the governing equations that were previously developed in Chapter IV must be experimentally measured or estimated from literature correlations. Based on industrial experimental conditions for the fixed-bed system (see Table IV in Chapter III) and literature correlations, numerical values of input model parameters are summarized in Table VII (for an example case of the sulfidation run) and in Table VIII (for an example case of the regeneration run). In Appendix A, procedures and example calculations estimating each parameter value, shown in Table VII, are described in detail.

In Table VII and Table VIII, operating temperatures, operating pressures, and the feed gas compositions (1.88 vol% of H_2S for the sulfidation; 2.5 vol% of O_2 for the regeneration) are directly or indirectly involved in obtaining numerical values of the physical properties (i.e., D_e , k_m , h , and C_{pg}) and other parameters. Reestimation of these parameters are required in the simulation runs under different operating conditions.

For parametric studies in this project, the ranges of operating temperatures for the sulfidation and the regeneration are varied from 600 to 800 K and from 550 to 850 K, respectively. The ranges of H_2S and O_2 concentrations for the sulfidation and the regeneration are varied from 1.88 to 4.0 vol% and from 1.5 to 2.5 vol%, respectively. The sulfidation and the regeneration are simulated at fixed operating pressures.

Literature correlations used in this work for the estimation of gas-solid mass transfer coefficients, gas-solid heat transfer coefficients, and effective diffusivity in the sorbent are briefly discussed as follows:

The gas-solid mass transfer coefficient (k_m) in fixed-beds is estimated by a correlation reported by Wakao and Funazkri (1978):

$$\text{Sh} = 2 + 1.1 \text{Sc}^{1/3} (\text{Re}_p)^{0.6}, \quad 3 < \text{Re}_p < 10,000 \quad (1)$$

where

$$\text{Sh} = \frac{k_m d_{pe}}{D_m} = \text{Sherwood number} \quad (2)$$

$$\text{Sc} = \frac{\mu}{\rho_g D_m} = \text{Schmidt number} \quad (3)$$

$$\text{Re}_p = \frac{\rho_g d_{pe} U}{\mu} = \text{particle Reynolds number} \quad (4)$$

In the above dimensionless numbers, D_m is the molecular diffusivity and it can be expressed as D_{AB} for binary gas systems. d_{pe} is an equivalent sorbent diameter. Other terms were previously defined.

The gas-solid heat transfer coefficient (h) in fixed-beds is estimated using the following correlations (when $2 < \text{Re}_p < 100$) suggested by Gliddon and Cranfield (1970):

$$\text{Nu or (Bi)}_h = 0.36(\text{Re}_p)^{0.94} \quad (5)$$

$$j_h = 0.41(\text{Re}_p)^{-0.06} \quad (6)$$

where

$$\text{Nu} = \frac{hd_{pe}}{k} = \text{Nusselt number} \quad (7)$$

$$\text{Pr} = \frac{C_{pg}\mu}{k} = \text{Prandtl number} \quad (8)$$

Here, k is a gas thermal conductivity. Correlations (5) and (6) are concerned with the total particle-fluid heat transfer (Doraiswamy and Sharma, 1984).

The effective diffusivity (D_e) in the sorbent is estimated by a modified correlation (by Wen, 1968) of the random pore model of Wakao and Smith (1962):

$$D_e = D_c(\varepsilon_p)^2 \quad (9)$$

where

$$\frac{1}{D_c} = \frac{1}{D_K} + \frac{1}{D_{AB}} \quad (10)$$

In Eqs. (9) and (10), D_c is a combined diffusivity from Knudsen diffusion and bulk diffusion. ϵ_p is the sorbent porosity.

The Knudsen diffusivity (D_K , cm^2/s) is obtained from the following equation:

$$D_K = 9,700 (r^*)(T/M)^{1/2} \quad (11)$$

where

r^* = mean pore radius, cm

T = temperature, K

M = molecular weight of gas

The bulk diffusivity (D_{AB} , cm^2/s) is estimated from the Chapman-Enskog equation (Reid et al., 1987):

$$D_{AB} = \frac{0.0026T^{3/2}}{P(M_{AB})^{1/2}(\sigma_{AB})^2\Omega_D} \quad (12)$$

where

T = temperature, K

P = pressure, bar

σ_{AB} = characteristic length, Angstroms

Ω_D = diffusion collision integral, demensionless

$$M_{AB} = 2[(1/M_A) + (1/M_B)]^{-1}$$

M_A, M_B = molecular weights of A and B

TABLE VII
MODEL PARAMETERS USED FOR SULFIDATION
(PILOT PLANT)

Reactor and sorbent details:

Bed diameter, D(cm)	167.6
Bed length, L(cm)	194.8
Bed voidage, ϵ_v	0.4
Sorbent radius, R(cm)	0.1588
Sorbent bulk density, ρ_s (g/cm ³)	1.121
Sorbent charge, w(g)	4.818 E+06

Operating conditions & kinetic parameters:

Temperature, T(K)	700
Pressure, P(atm)	1.05
Superficial gas velocity, U(cm/h)	1.04 E+05
Volumetric gas flow rate, v(cm ³ /h)	2.294 E+09
Initial conc. of H ₂ S, C _{Abo} (mol/cm ³)	3.437 E-07
Initial conc. of ZnO, C _{B0} (mol/cm ³)	0.0115
Heat of reaction, ΔH (cal/mol)	- 1.462 E+04
Intrinsic reaction rate constant at shrinking core surface, k _s (cm ⁴ /mol·h)	4.0 E+08
Stoichiometric coefficient, b	1.0

Physical properties:

Effective diffusivity within the sorbent, D _e (cm ² /h)	59.96
Gas-solid mass transfer coefficient, k _m (cm/h)	38,430
Gas-solid heat transfer coefficient, h(cal/cm ² ·h·K)	9.036
Average heat capacity of gas, C _{pg} (cal/g·K)	0.2691
Average heat capacity of solid, C _{ps} (cal/g·K)	0.2078

TABLE VIII
MODEL PARAMETERS USED FOR REGENERATION
(PILOT PLANT)

Reactor and sorbent details:	
Bed diameter, D(cm)	167.6
Bed length, L(cm)	194.8
Bed voidage, ϵ_v	0.4
Sorbent radius, R(cm)	0.1588
Sorbent bulk density, ρ_s (g/cm ³)	1.121
Sorbent charge, w(g)	4.818 E+06
Operating conditions & kinetic parameters:	
Temperature, T(K)	700
Pressure, P(atm)	1.6
Superficial gas velocity, U(cm/h)	8.95 E+04
Volumetric gas flow rate, v(cm ³ /h)	1.975 E+09
Initial conc. of O ₂ , C _{Ab0} (mol/cm ³)	6.964 E-07
Initial conc. of ZnS, C _{B0} (mol/cm ³)	2.035 E-02
Heat of reaction, ΔH (cal/mol)	- 1.099 E+05
Intrinsic reaction rate constant at shrinking core surface, k_s (cm ⁴ /mol·h)	4.0 E+08
Stoichiometric coefficient, b	0.667
Physical properties:	
Effective diffusivity within the sorbent, D _e (cm ² /h)	61.78
Gas-solid Mass transfer coefficient, k _m (cm/h)	35,610
Gas-solid heat transfer coefficient, h(cal/cm ² ·h·K)	7.692
Average heat capacity of gas, C _{pg} (cal/g·K)	0.2568
Average heat capacity of solid, C _{ps} (cal/g·K)	0.1949
wt% sulfur loading, wt(%)	32.9

CHAPTER VII

RESULTS AND DISCUSSIONS

In this Chapter, the performance of a mathematical model developed for the description of an adiabatic fixed-bed sulfidation-regeneration system for tail gas clean-up is discussed, based on simulation results for a lab-scale system and a pilot plant scale system, respectively. For the lab-scale system, the effects of various parameters on the H₂S breakthrough curves, gas temperature profiles and sulfur loading profiles (for the regeneration case) are additionally presented from simulation results.

Laboratory-scale Tail gas Clean-up System

Results from the Sulfidation Simulation

Numerical values of model parameters for this simulation case are shown in Table IX. Figure 12 shows a predicted H₂S breakthrough curve for the complete sulfidation of fresh ZnO/Al₂O₃ sorbents in the adiabatic fixed-bed reactor. Computed data for sulfidation time versus effluent H₂S concentration is listed in Appendix C. In this figure, the corresponding breakthrough time is 9.6 hr when effluent H₂S concentration from the sulfidation reactor is 30 ppmv. Elapsed time for the complete sulfidation of the fresh bed is 16.2 hr. For Claus tail gas clean-up, the operation of the sulfidation reactor should be stopped at (or just before) the breakthrough time (for example, 9.6 hr). Figure 13 shows

TABLE IX
MODEL PARAMETERS FOR
THE SULFIDATION

Reactor and sorbent details:

Bed diameter, D(cm)	4.09
Bed length, L(cm)	19.48
Bed voidage, ϵ_v	0.4
Sorbent radius, R(cm)	0.1588
Sorbent bulk density, ρ_s (g/cm ³)	1.121
Sorbent charge, w(g)	286.9

Operating conditions & kinetic parameters:

Temperature, T(K)	700
Pressure, P(atm)	1.05
Superficial gas velocity, U(cm/h)	3.119 E+04
Volumetric gas flow rate, v(cm ³ /h)	4.098 E+05
Initial conc. of H ₂ S, C _{Ab0} (mol/cm ³)	3.437 E-07
Initial conc. of ZnO, C _{B0} (mol/cm ³)	0.0115
Heat of reaction, ΔH (cal/mol)	- 1.462 E+04
Intrinsic reaction rate constant at shrinking core surface, k_s (cm ⁴ /mol·h)	4.0 E+08
Stoichiometric coefficient, b	1.0

Physical properties:

Effective diffusivity within the sorbent, D _e (cm ² /h)	59.93
Gas-solid mass transfer coefficient, k _m (cm/h)	21,980
Gas-solid heat transfer coefficient, h(cal/cm ² ·h·K)	2.914
Average heat capacity of gas, C _{pg} (cal/g·K)	0.2691
Average heat capacity of solid, C _{ps} (cal/g·K)	0.2078

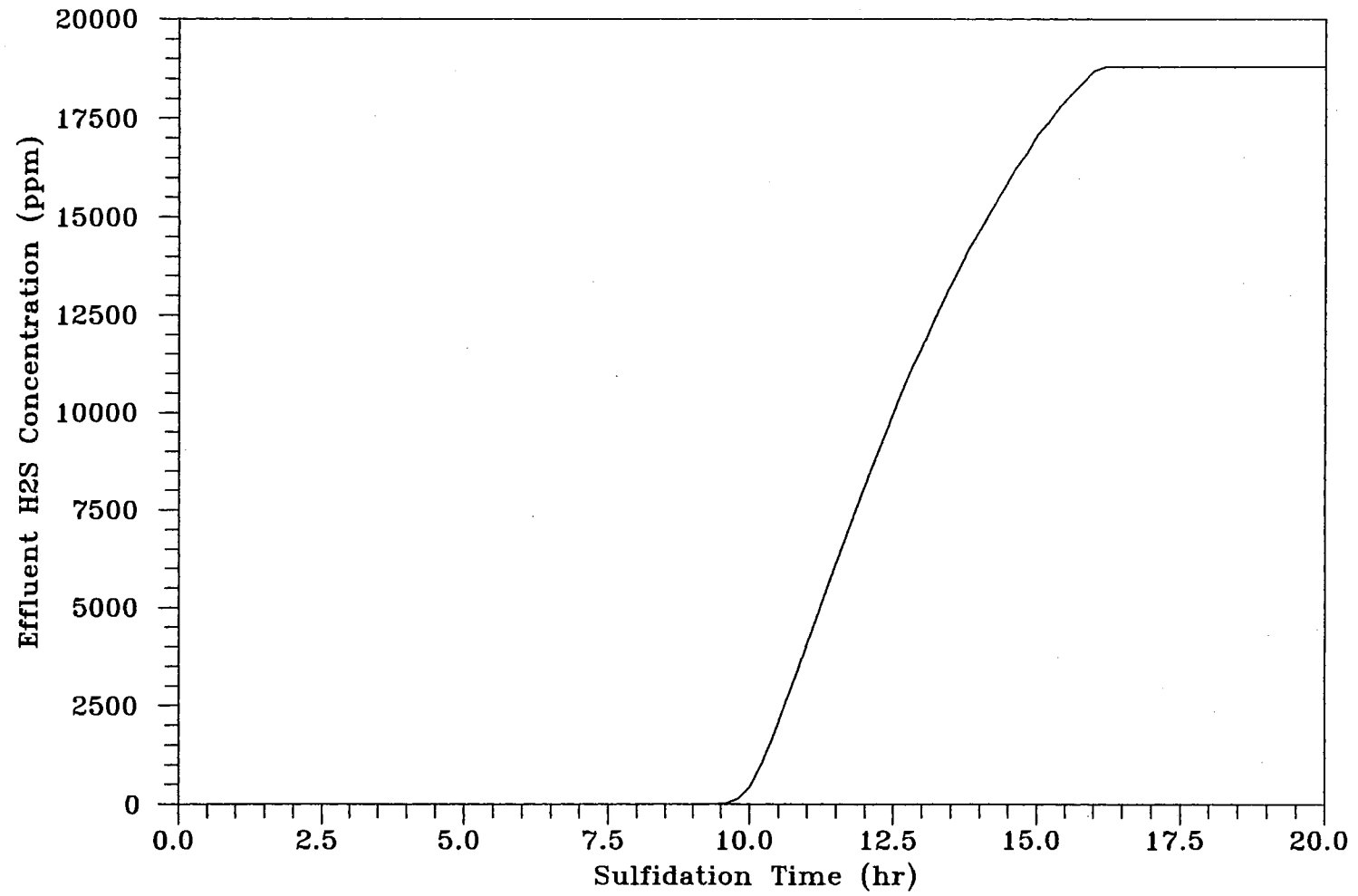


Figure 12. Breakthrough Curve for Sulfidation

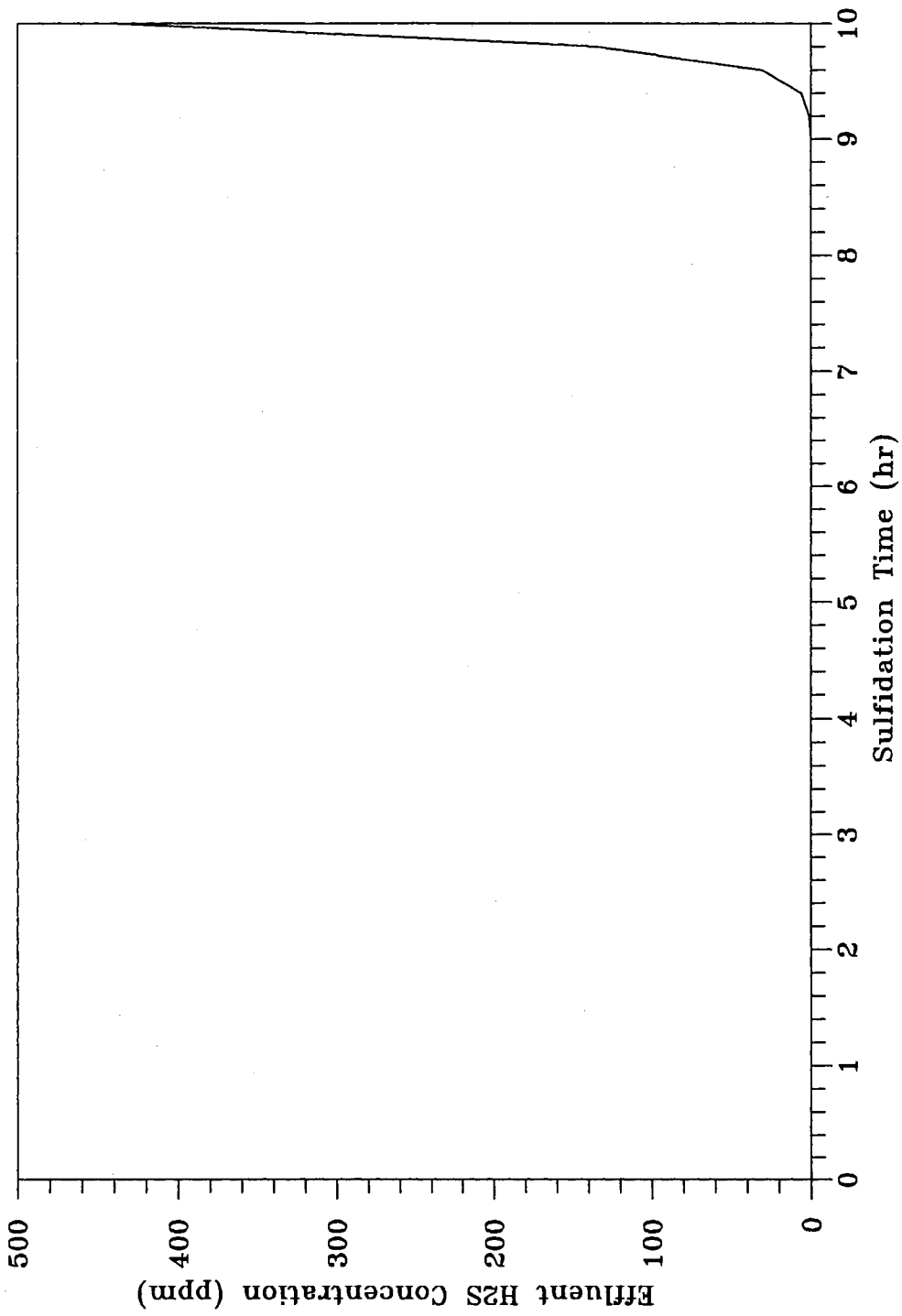


Figure 13. Breakthrough Curve for Sulfidation (at breakthrough time)

the breakthrough curve around this breakthrough time.

Figure 14 shows dimensionless H_2S concentration profiles in the sulfidation reactor (at sulfidation times from 1 to 10 hours). After about 4 hours, the sulfidation reaction fronts showing the same shape are traveling along the fixed-bed. The breakthrough occurs between the reaction front at 9 hr and that at 10 hr. In Figure 14, slowly decaying concentration profiles are observed. More sharply decaying concentration profiles are preferred in the operation of a commercial-type sulfidation reactor (for better utilization of the sorbents in the fixed-bed reactor). Figure 43 shows sharply decaying concentration profiles observed in the pilot plant scale sulfidation reactor.

Figure 15 shows the sorbent conversion profiles in the sulfidation reactor (at sulfidation times from 1 to 10 hours). ZnO/Al_2O_3 sorbents at the fixed-bed inlet are completely converted to ZnS/Al_2O_3 after about 4 hours of sulfidation. The same shape of sorbent conversion profiles are obtained once the sorbents in the entrance of the fixed-bed is completely converted. At breakthrough, the average conversion of the sorbents in the bed is 76.57 %. The sorbent conversion value at breakthrough time for each grid point along the reactor axis is presented in Appendix C. This conversion information will be used for the computation of initial sulfur loading profile for the regeneration.

Figure 16 shows the sulfur loading profiles in the sulfidation reactor (at times from 1 to 10 hours). In this figure, the sulfur loading is defined as weight of loaded sulfur per weight of sulfided sorbent (i.e., gram of sulfur/gram of ZnS sorbent). Based on this definition, the maximum sulfur loading shown in Figure 16 is 0.3284. From the stoichiometric equation of the sulfidation reaction, the maximum sulfur loading of fresh sorbent can be defined as weight of loaded sulfur per weight of fresh sorbent (i.e., gram of sulfur/ gram of ZnO sorbent).

Figure 17 shows dimensionless gas temperature profiles in the sulfidation reactor at times from 0.1 to 0.5 hour. At $t = 0.2$ hr, maximum temperature rise of

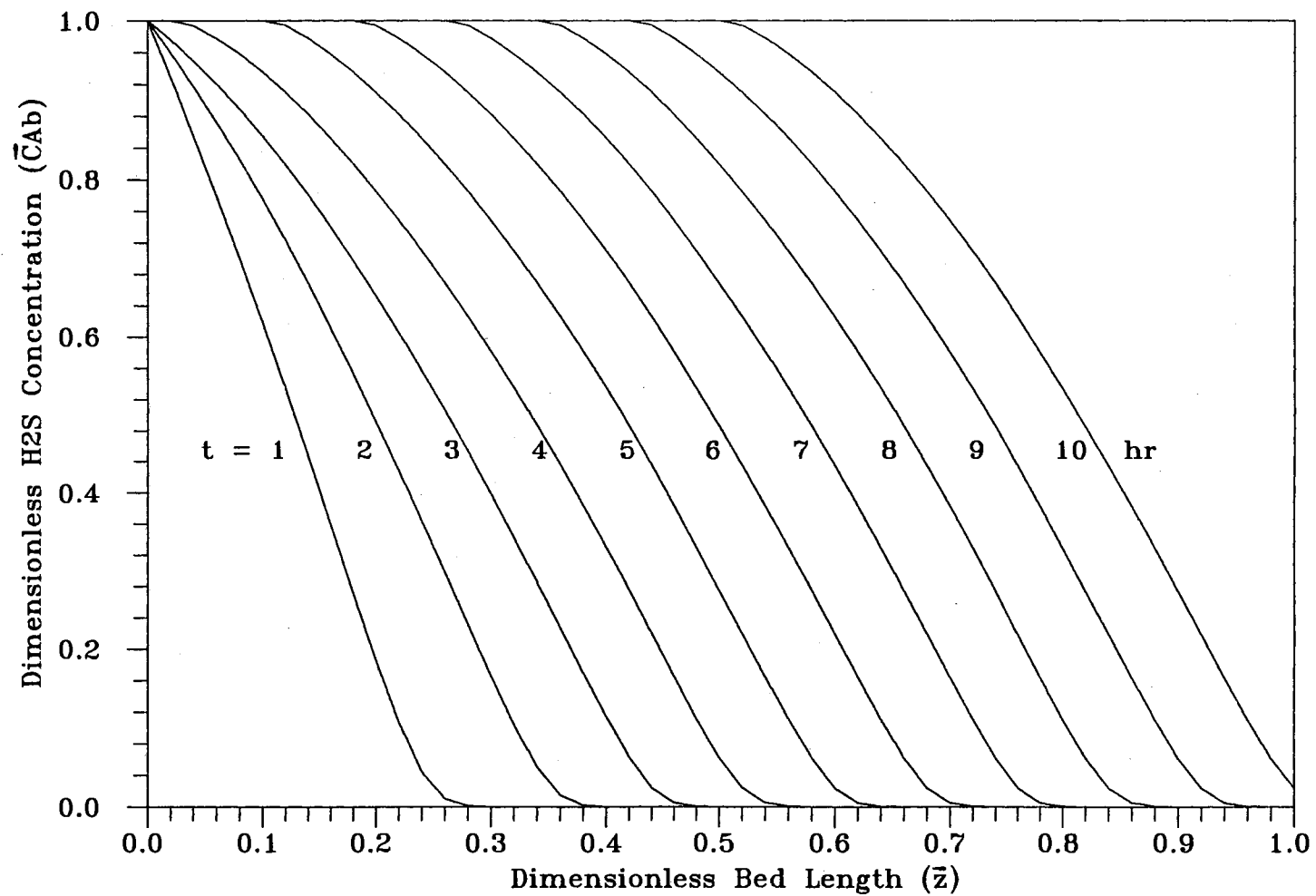


Figure 14. Dimensionless H₂S Concentration Profiles for Sulfidation

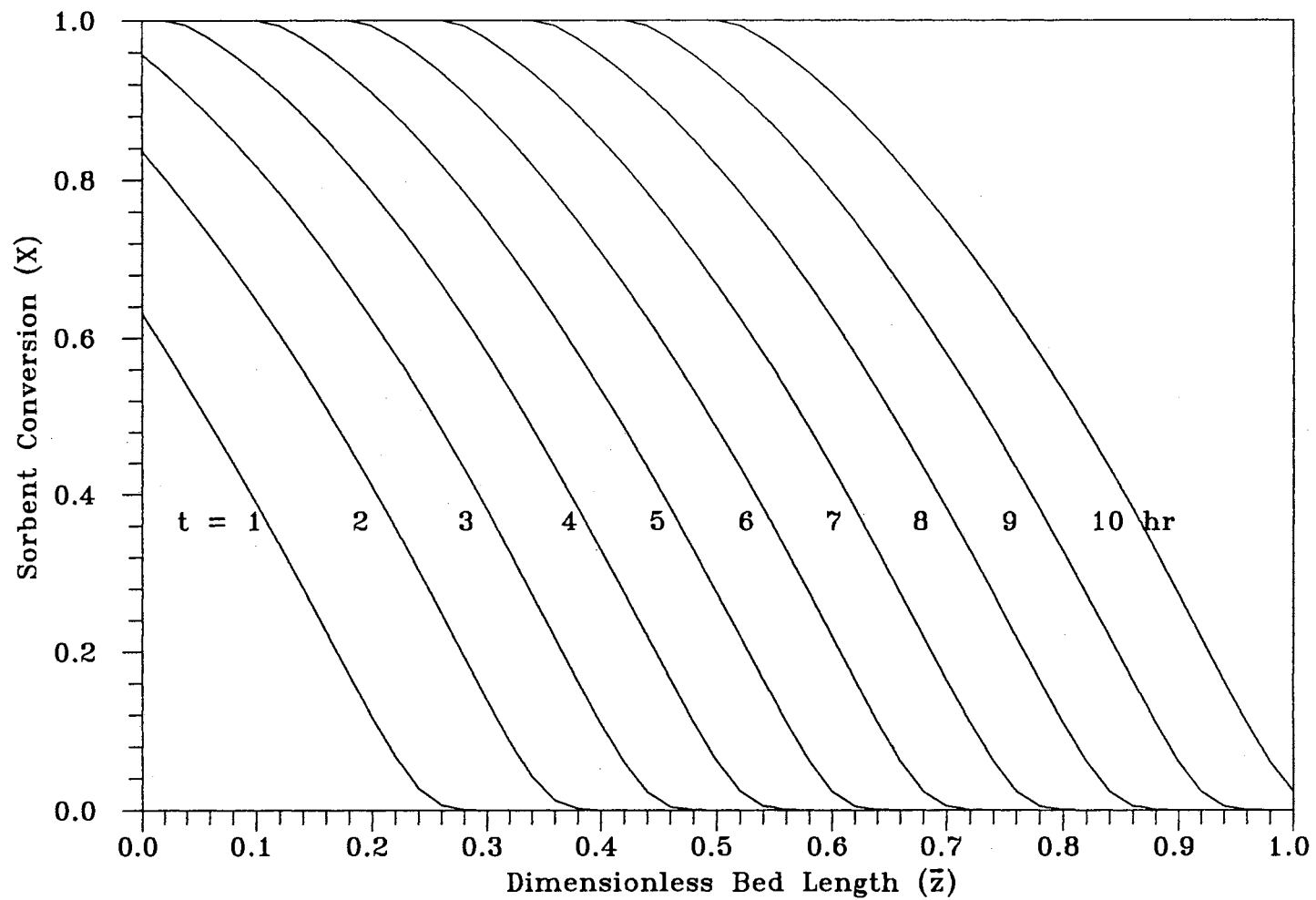


Figure 15. Sorbent Conversion Profiles for Sulfidation

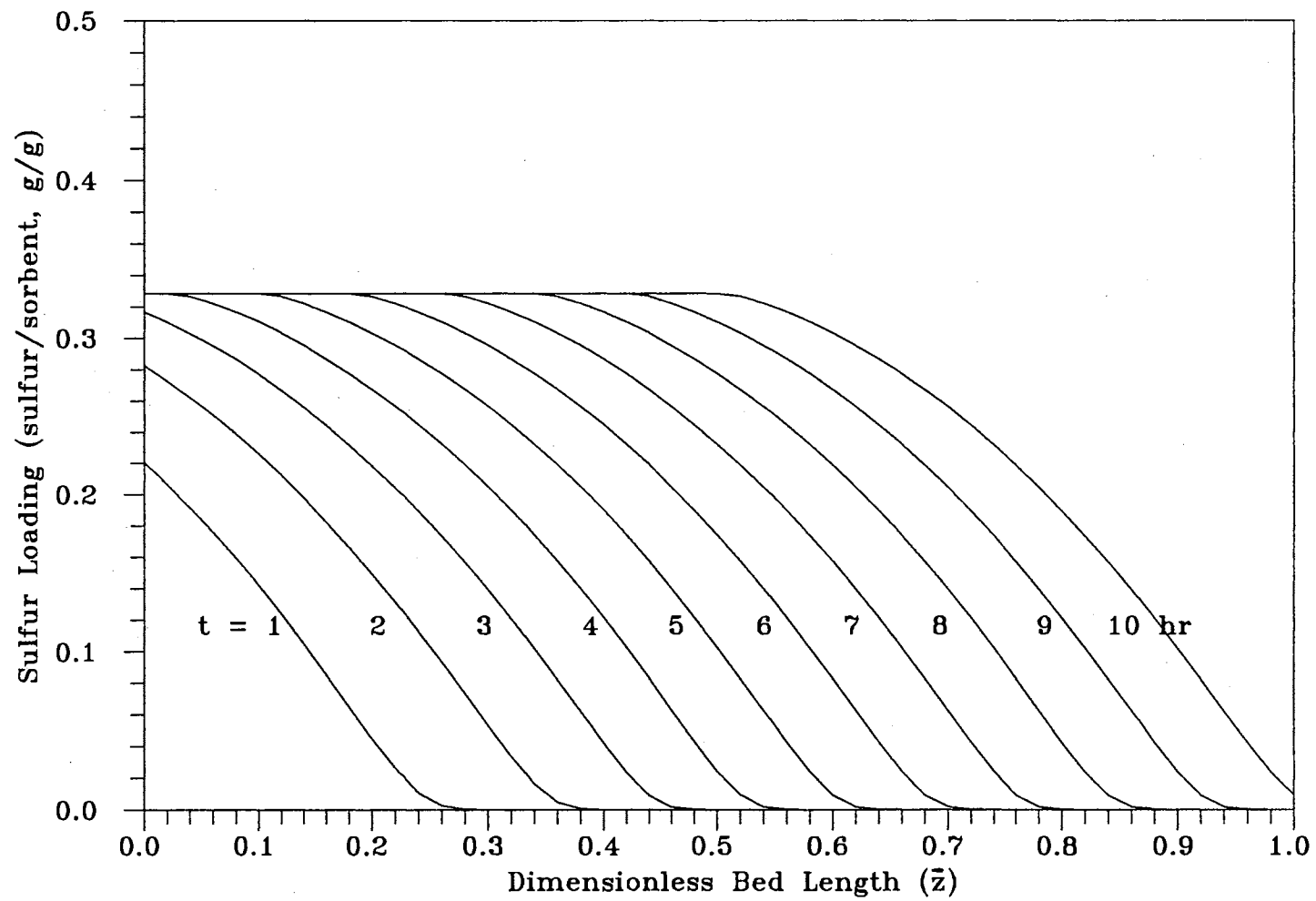


Figure 16. Sulfur Loading Profiles for Sulfidation

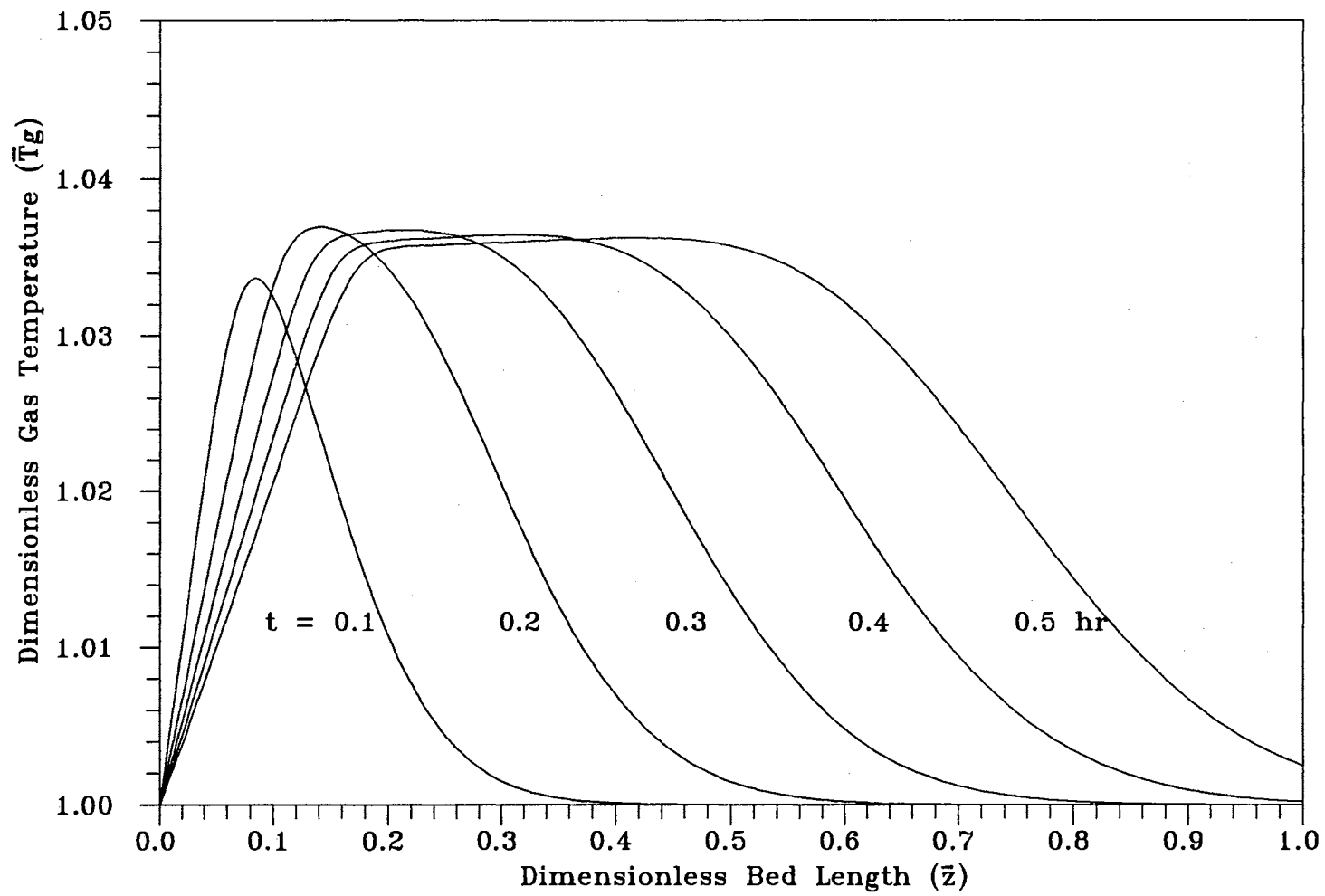


Figure 17. Dimensionless Gas Temperature Profiles for Sulfidation

25.9 K occurs at the bed position $z = 0.114$. Unsteady state gas temperature profiles are shown in this figure. The traveling of temperature profiles haven't started yet as the sorbents in the entrance region of the fixed-bed are still under sulfidation reaction.

Complete sulfidation of sorbents in this region occurs at about $t = 4$ hr.

Figure 18 presents dimensionless gas and sorbent temperature profiles at $t = 0.1$, 0.2 and 0.5 hour. From the temperature profiles at $t = 0.1$ hr, the temperature difference between the gas and the sorbent is about 2.6 K when the sorbent reaches to the maximum point. From the temperature profiles at $t = 0.2$ hr, the temperature difference between them is about 1.2 K. In this figure, before the sorbent temperature reaches to the maximum point, the temperature of the sorbent is higher than that of the gas. This phenomena explains that the sulfidation reaction proceeds actively before this point. However, after this point (i.e., in inactive reaction region), the gas temperature is higher than that of the sorbent because gas transports heat from active reaction region to inactive reaction region.

Figure 19 shows dimensionless gas temperature profiles in the reactor at different sulfidation times ($t = 1, 5, 9$ and 11 hours). At $t = 1$ hr, the entrance region of the fixed-bed is still under sulfidation reaction. At this time, the gas temperature approaches to an asymptotic value from about $z = 0.28$. At $t = 5$ hr, the sorbents in the first 10 % of the reactor have completed the reaction and the gas temperature profile has already started traveling down the bed. Figure 20 presents dimensionless gas and sorbent temperature profiles in the reactor. At $t = 1$ hr, the sorbent temperature also approaches to the asymptotic value from about $z = 0.28$. Sorbent temperatures are higher than gas temperatures until the gas and sorbent temperatures approach the asymptotic value.

In the following paragraphs, the effects of various parameters on the H_2S breakthrough curves are discussed. Although the sulfidation reaction is stopped at (or just before) breakthrough in the operation of a tail gas clean-up system, the breakthrough curve showing complete sulfidation of the sorbent in the fixed-bed is

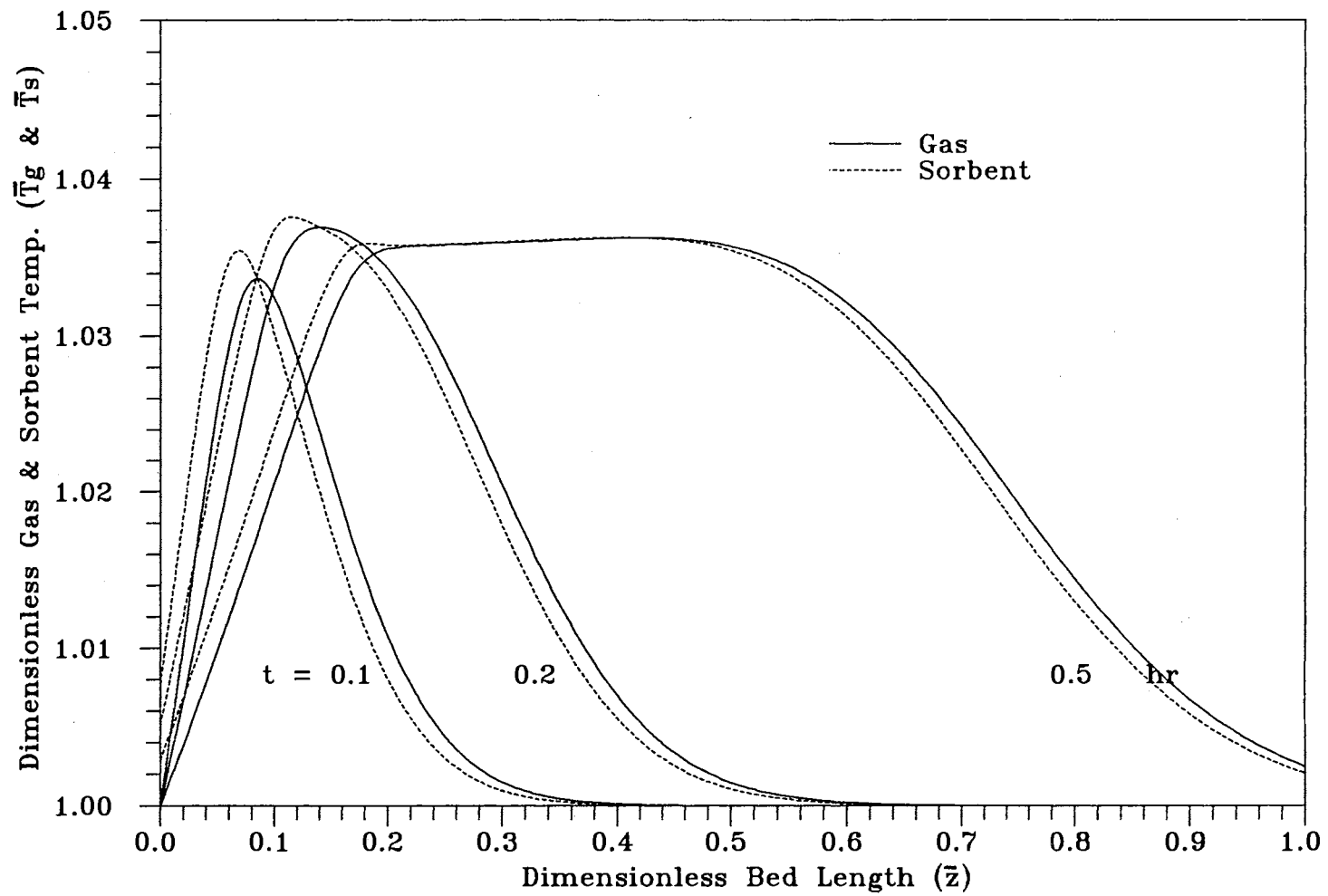


Figure 18. Dimensionless Gas & Sorbent Temperature Profiles for Sulfidation

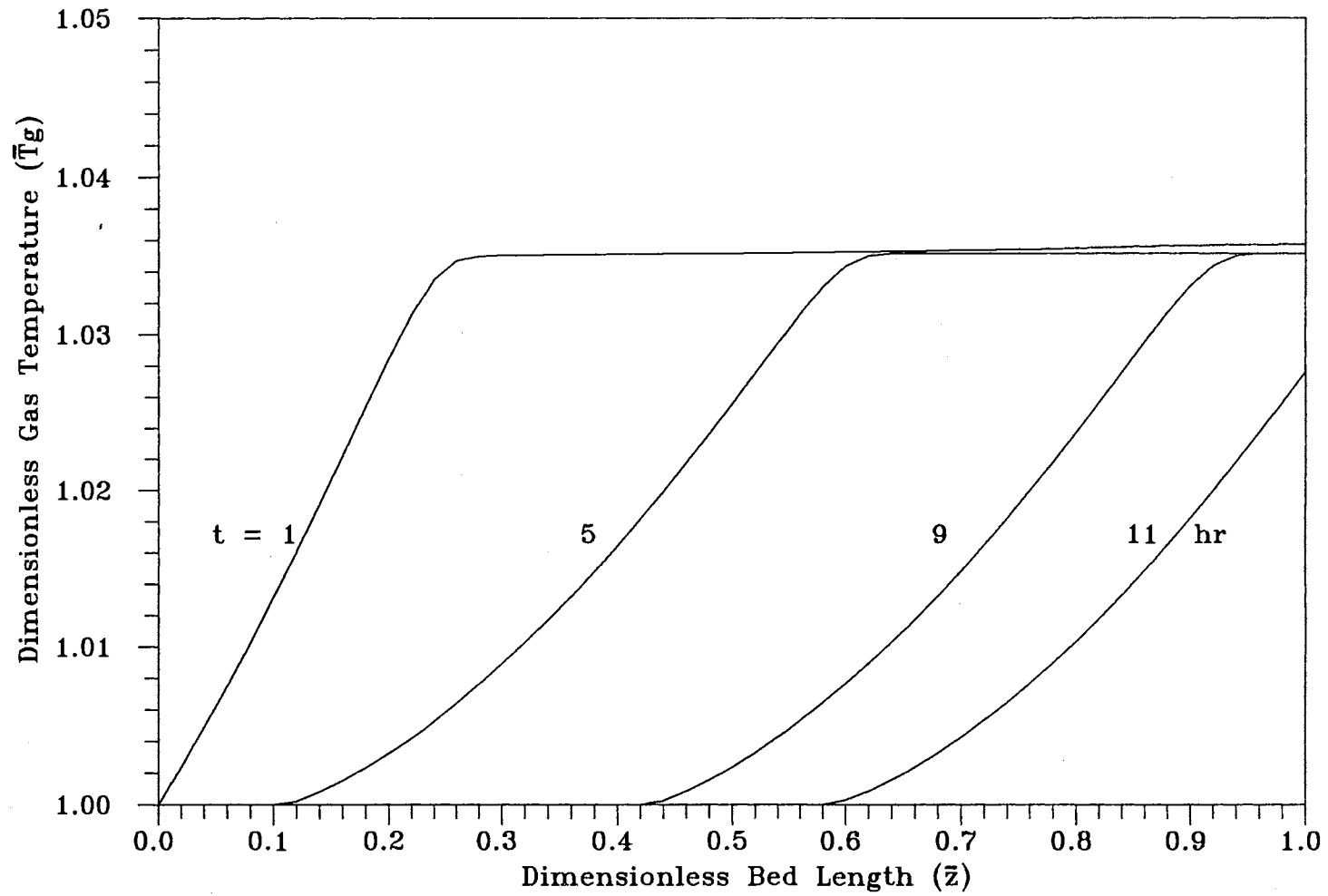


Figure 19. Dimensionless Gas Temperature Profiles for Sulfidation (from 1 to 11 hr)

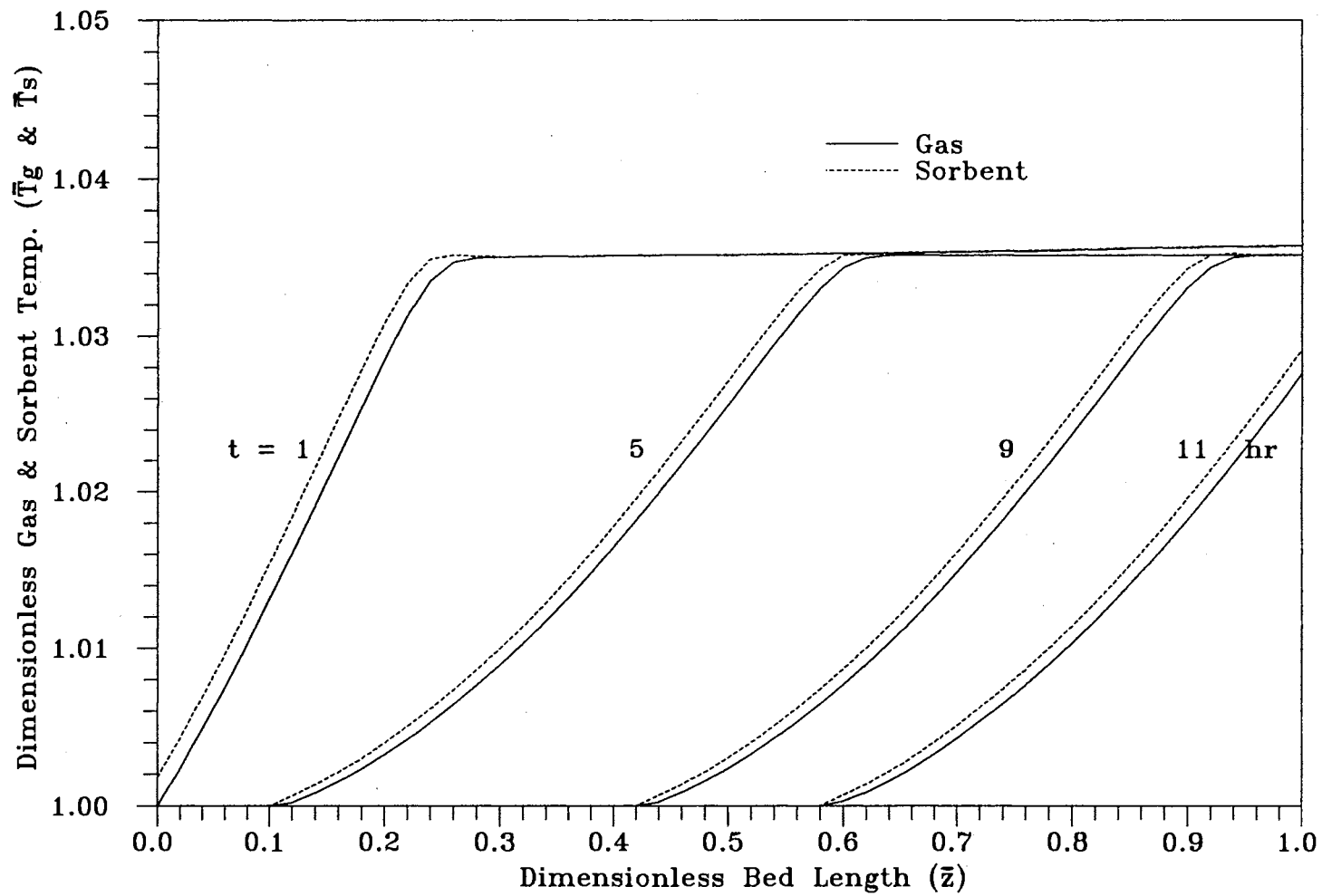


Figure 20. Dimensionless Gas & Sorbent Temperature Profiles for Sulfidation (from 1 to 11 hr)

discussed because this curve can describe the general characteristics occurring in the reactor.

The effect of inlet H_2S concentration on the sulfidation breakthrough is shown in Figure 21. With all other conditions remaining the same, an increase in the inlet H_2S concentration shows faster breakthrough time (for the same breakthrough concentration of 30 ppmv). When the inlet H_2S concentrations are 1.18, 3.0 and 4.0 mol %, the predicted breakthrough times are 9.6, 5.98 and 4.47 hours, respectively. With the higher inlet H_2S concentration, a shorter time span spent from the breakthrough to the complete sulfidation is obtained. This result represents the strong effect of the inlet H_2S concentration (or mole fraction) on the global reaction rate in the reactor.

The effect of inlet gas temperature on the sulfidation breakthrough curve is shown in Figure 22. When inlet gas temperatures used in the simulation are 600, 700 and 800 K, predicted breakthrough times are 9.68, 9.60 and 9.51 hours, respectively. Appreciable change of breakthrough time with respect to inlet gas temperature is not observed. A weak influence of sulfidation temperature on the experimental data was reported in fixed-bed experiments of other sulfidation studies by Yumura and Furimsky (1985) and Efthimiadis and Sotirchos (1993). Zinc oxide sorbents were used in their studies. Trends shown in Figure 22 are in agreement with their experimental studies.

The effect of superficial gas velocity on the sulfidation breakthrough curve is shown in Figure 23. With the operating temperature and inlet H_2S concentration kept constant, only the superficial gas velocity was varied in the simulation. A higher superficial velocity gives an earlier breakthrough time for the constant breakthrough concentration. At $U = 11.55$ cm/sec, for example, the predicted breakthrough time is 6.84 hour. At $U = 8.66$ cm/sec (i.e., 75 % of the previous superficial velocity, 11.55 cm/sec), the predicted breakthrough time is 9.60 hour. However, the slope of the breakthrough curve (i.e., the global rate of the reaction) is almost identical.

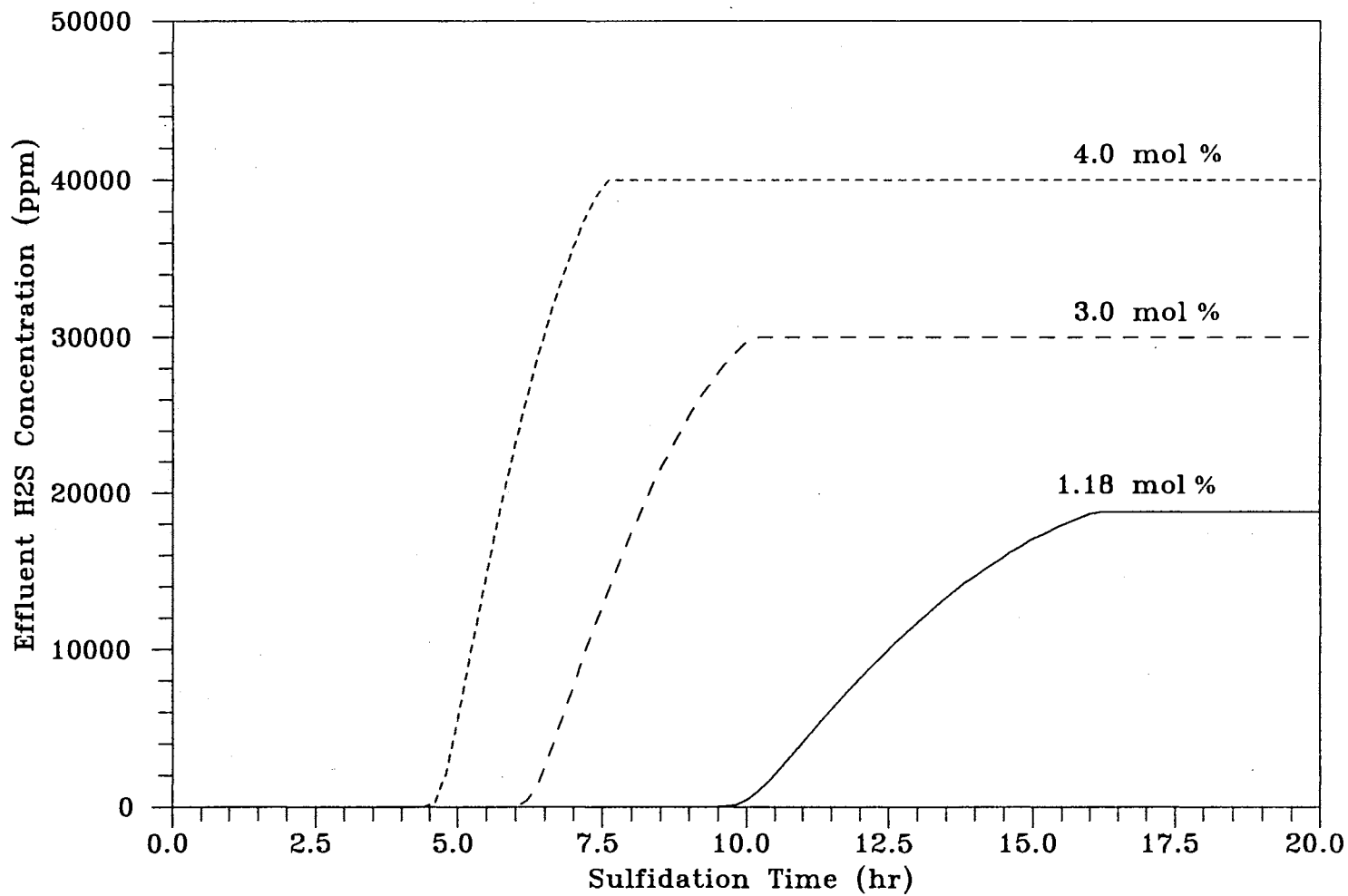


Figure 21. Effect of Inlet H₂S Concentration on Sulfidation Breakthrough curve

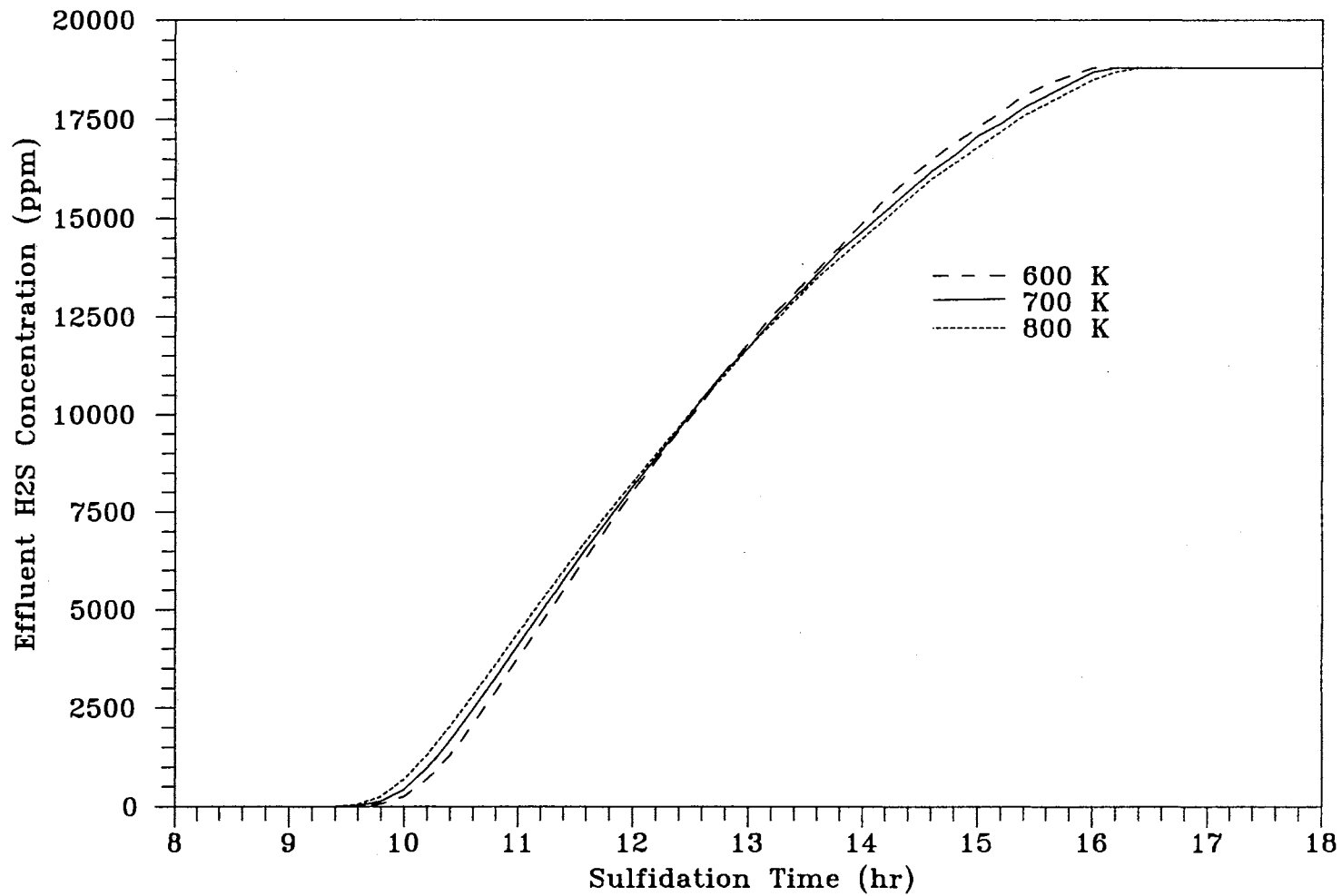


Figure 22. Effect of Inlet Gas Temperature on Sulfidation Breakthrough Curve

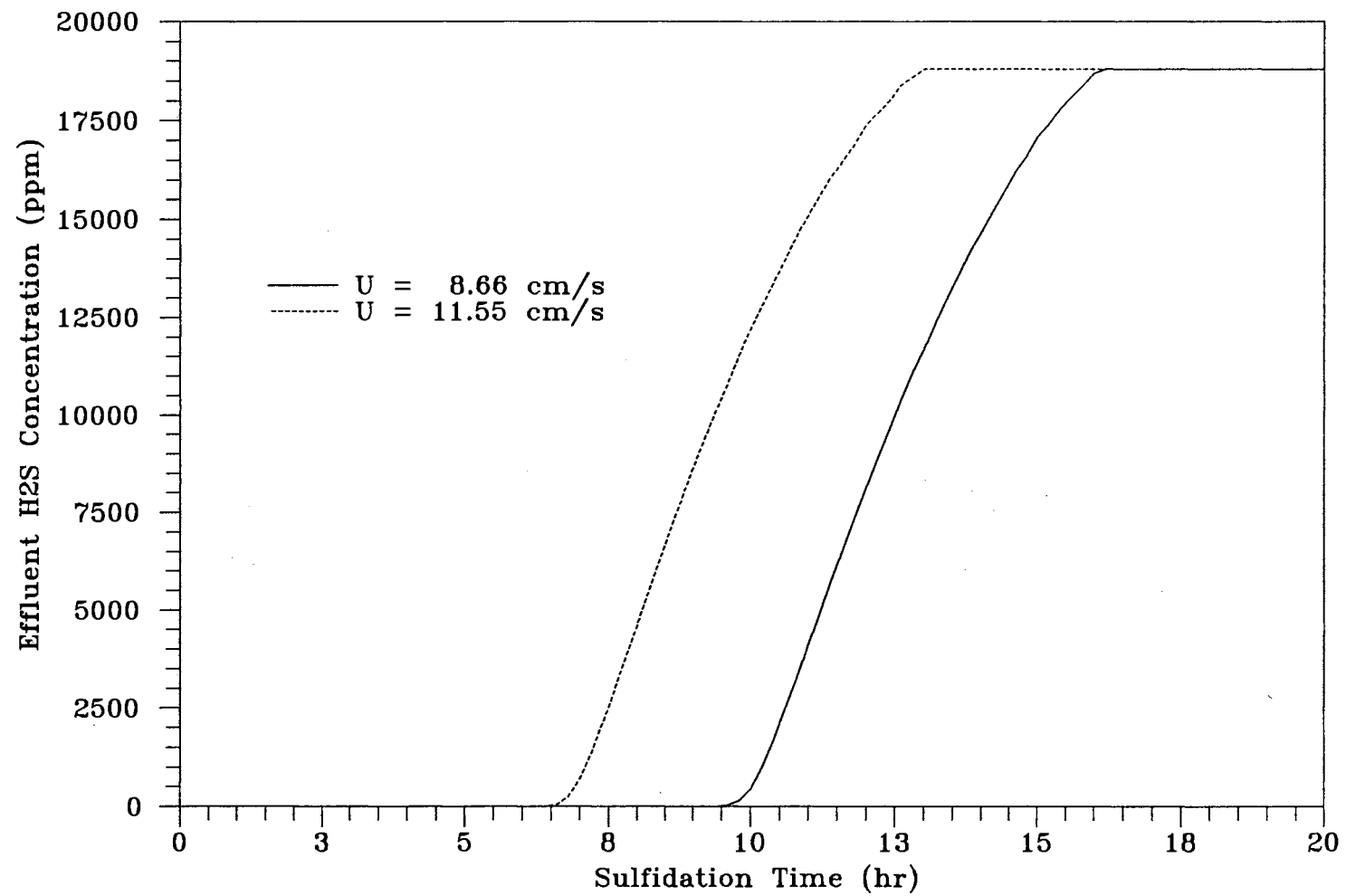


Figure 23. Effect of Superficial Gas Velocity on Sulfidation Breakthrough Curve

Results from the Regeneration Simulation

Figure 24 shows the initial sulfur loading profile as a function of dimensionless fixed-bed length. This profile represents the loading status of ZnS/Al₂O₃ sorbents in the adiabatic fixed-bed regenerator at the time of starting the regeneration reaction. Computation of this profile is described as follows: In the proposed tail gas clean-up fixed-bed system, the operation of the sulfidation reactor is stopped at a preset breakthrough concentration. Corresponding H₂S breakthrough concentration is 30 ppmv in this study. The sulfur loading along the sulfidation reactor axis at this breakthrough time is readily computed from the sorbent conversion data. However, in the operation the regenerator, the O₂ gas flow direction is opposite to that of the sulfidation gas flow. Thus, the profile shown in Figure 24 is just the reverse (with respect to the sulfidation reactor axis direction) of the sulfur loading profile at sulfidation breakthrough time.

Figure 25 shows the O₂ breakthrough curve for the complete regeneration of ZnS/Al₂O₃ sorbents in the adiabatic fixed-bed regenerator. Input model parameters for this regeneration simulation case is given in Table X. Time for the complete regeneration of these partially sulfided sorbents (from the previous sulfidation step) is 7.2 hr. If a fully sulfided bed is used for the regeneration, the computed time for the complete regeneration of the bed is 9.0 hr (not shown in this Figure).

Figure 26 shows the effluent SO₂ concentration profile from the regenerator for the complete regeneration of the partially sulfided bed. When the effluent SO₂ concentration from the regenerator reaches a preset value (i.e., 1000 ppmv in this study; Corresponding regeneration time is 6.75 hr.), the operation of the regenerator is stopped. In a real run of the regenerator for tail gas clean-up, produced SO₂ is recycled back to the Claus bed for additional sulfur recovery in Claus plants. Thus, the decision of a preset value for effluent SO₂ concentration is a crucial factor in the operation of the regenerator and depends on the operating policy of the Claus plants.

TABLE X
MODEL PARAMETERS FOR
THE REGENERATION

Reactor and sorbent details:

Bed diameter, D(cm)	4.09
Bed length, L(cm)	19.48
Bed voidage, ϵ_v	0.4
Sorbent radius, R(cm)	0.1588
Sorbent bulk density, ρ_s (g/cm ³)	1.121
Sorbent charge, w(g)	286.9

Operating conditions & kinetic parameters:

Temperature, T(K)	700
Pressure, P(atm)	1.6
Superficial gas velocity, U(cm/h)	2.685 E+04
Volumetric gas flow rate, v(cm ³ /h)	3.528 E+05
Initial conc. of H ₂ S, C _{Abo} (mol/cm ³)	6.964 E-07
Initial conc. of ZnO, C _{Bo} (mol/cm ³)	8.790 E-03
Heat of reaction, ΔH (cal/mol)	- 1.099 E+05
Intrinsic reaction rate constant at shrinking core surface, k_s (cm ⁴ /mol·h)	4.0 E+08
Stoichiometric coefficient, b	0.667

Physical properties:

Effective diffusivity within the sorbent, D _e (cm ² /h)	61.70
Gas-solid mass transfer coefficient, k _m (cm/h)	20,510
Gas-solid heat transfer coefficient, h(cal/cm ² ·h·K)	2.481
Average heat capacity of gas, C _{pg} (cal/g·K)	0.2568
Average heat capacity of solid, C _{ps} (cal/g·K)	0.1949
wt% sulfur loading, wt%	32.9

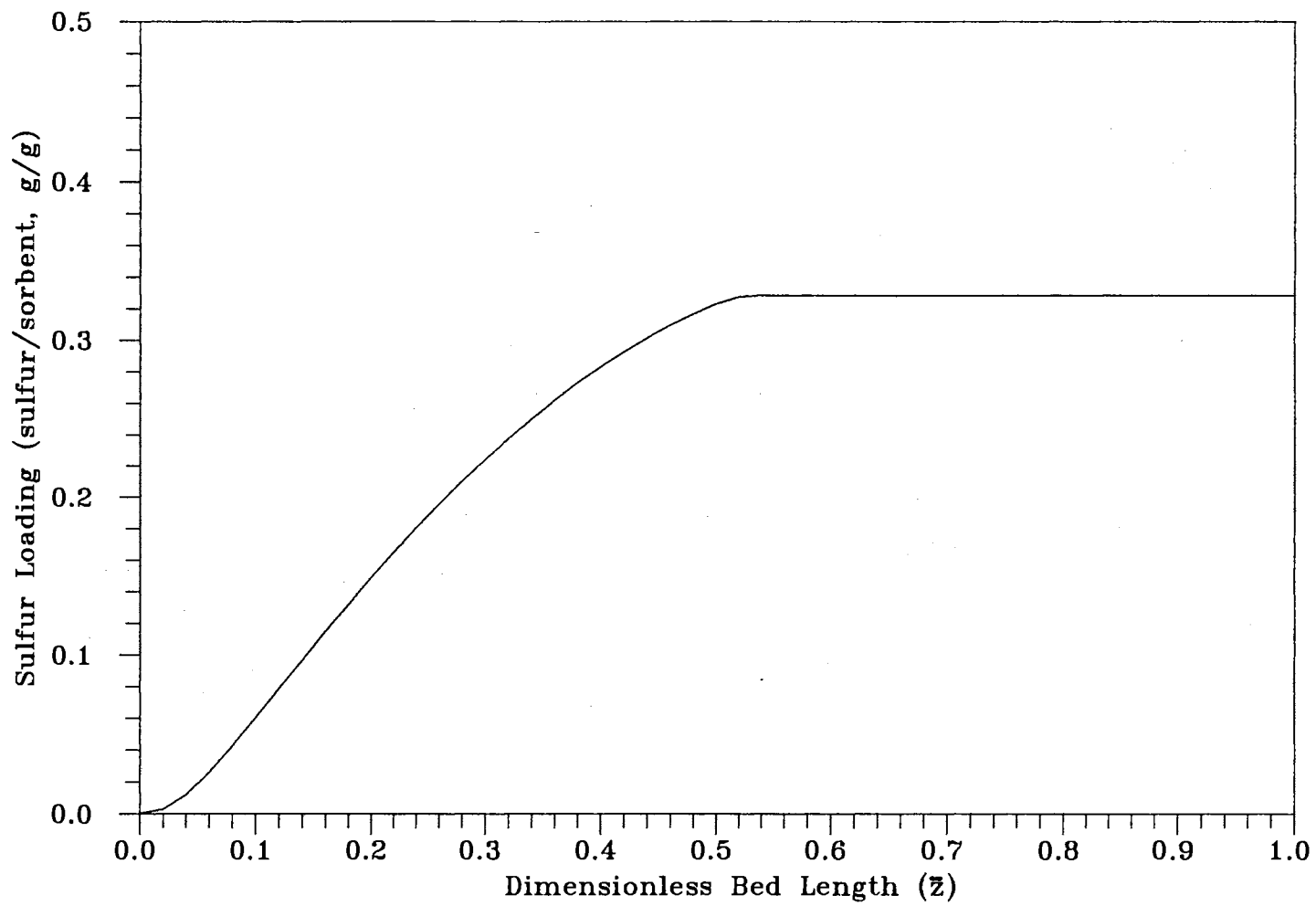


Figure 24. Initial Sulfur Loading Profile
for Regeneration

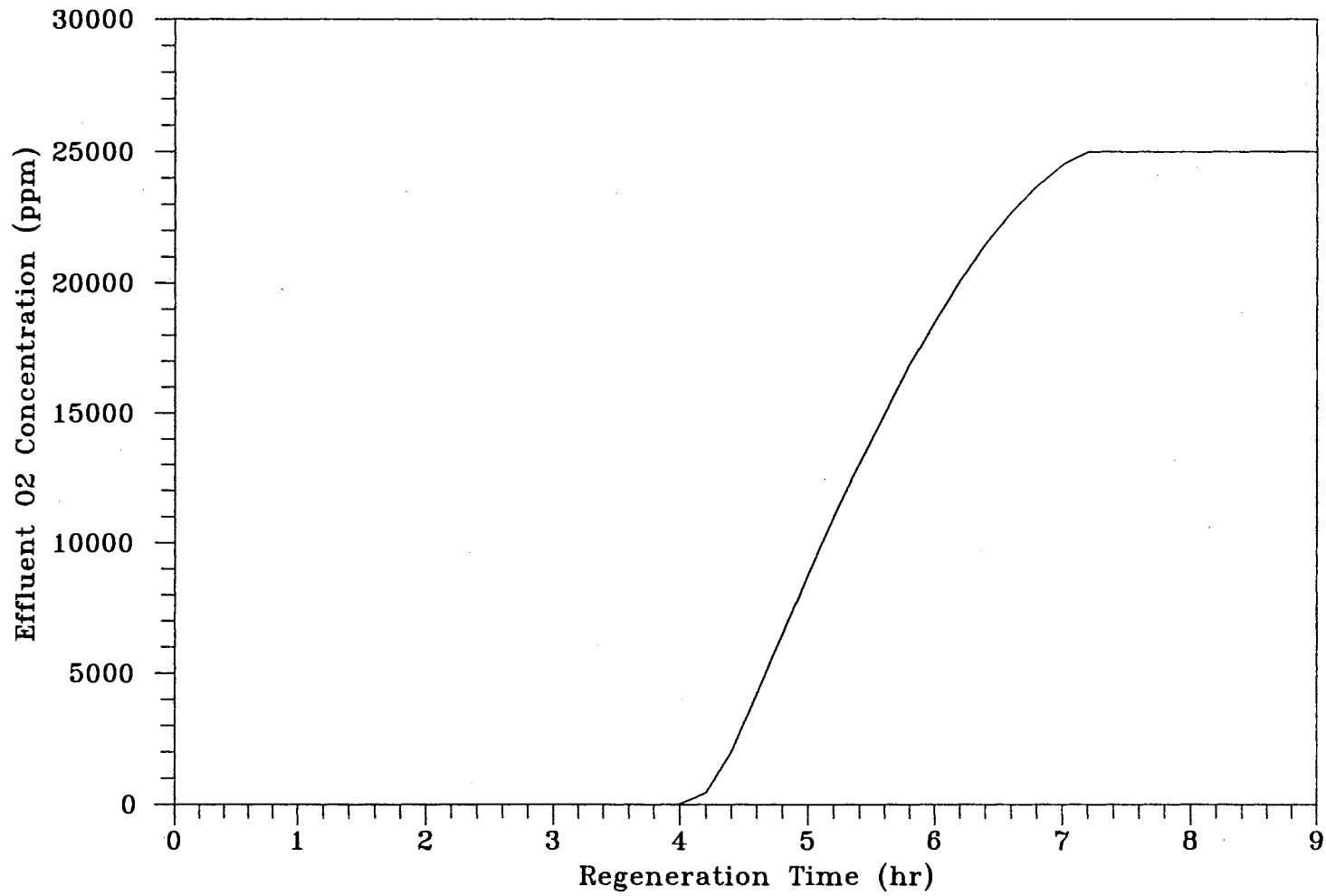


Figure 25. Breakthrough Curve for Regeneration

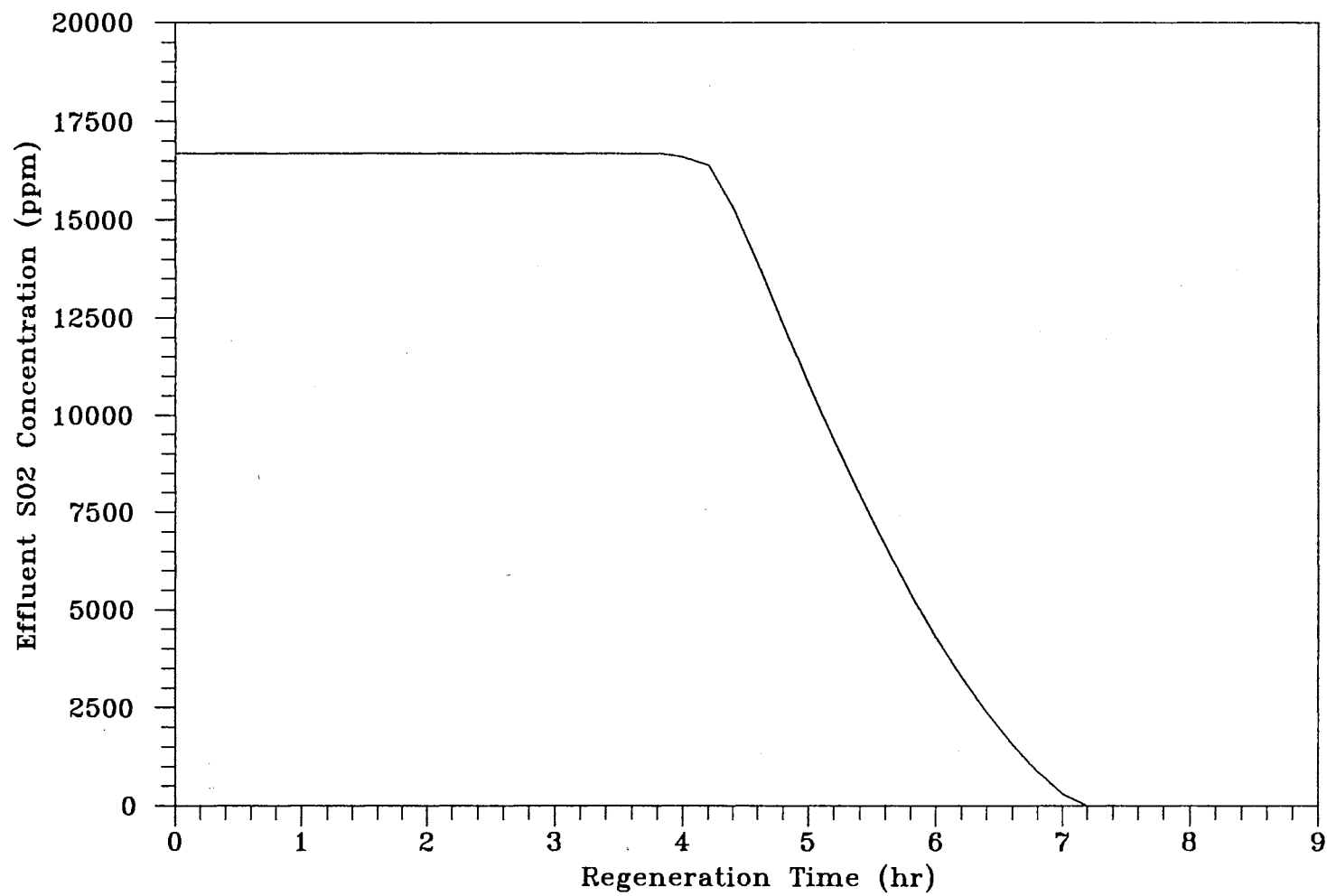


Figure 26. Effluent SO2 Concentration Profile for Regeneration

Effluent O_2 and SO_2 concentration profiles as a function of regeneration time are compared in Figure 27.

Figure 28 shows sulfur loading profiles in the regenerator (at times from 0 to 6 hours). The initial sulfur loading profile is represented by a dotted line. At $t = 1$ hr, about the first 26 % of the bed has been completely regenerated. At $t = 6$ hr, about the first 84 % of the fixed-bed has been completely regenerated.

Figure 29 shows dimensionless gas temperature profiles for regeneration (at times from 0.1 to 0.5 hr). After about 6 min. passed, the unsteady state gas temperature profiles start traveling along the regenerator. The early start of traveling phenomena is different from that for the sulfidation reactor simulation case since partially sulfided sorbents (i.e., small amount of ZnS reactants for regeneration) exist in the inlet region of the regenerator. When $t = 0.3$ hr, the gas temperature reaches to 1132 K at $z = 0.288$. In this case, the gas temperature rise was computed as 432 K, compared with the inlet gas temperature of 700 K.

Figure 30 shows dimensionless gas and sorbent temperature profiles for regeneration (at times from 0.1 to 0.5 hr). As in the case for the sulfidation, predicted sorbent temperatures were higher than those of the gas in the active reaction region. After the sorbent temperature reaches to the peak point, the gas temperature exceeds the sorbent temperature. When $t = 0.3$ hr, the highest sorbent temperature (i.e., 1140 K) was obtained at $z = 0.268$. In this case, the computed sorbent temperature rise was 440 K. When $t = 0.1$ hr, the maximum temperature difference between the gas and sorbent (i.e., 50 K) was obtained at $z = 0.132$. The temperature profiles shown in Figure 30 (or 29) represent typical characteristics of the highly exothermic regeneration reaction.

Figure 31 shows dimensionless gas temperature profiles in the regenerator at different times from 1 to 6 hr. After one hour passed, gas temperatures in the region near the fixed-bed outlet are higher than those at the early section of the fixed-bed since more ZnS reactants are available in the outlet region. Similar trends are also found for

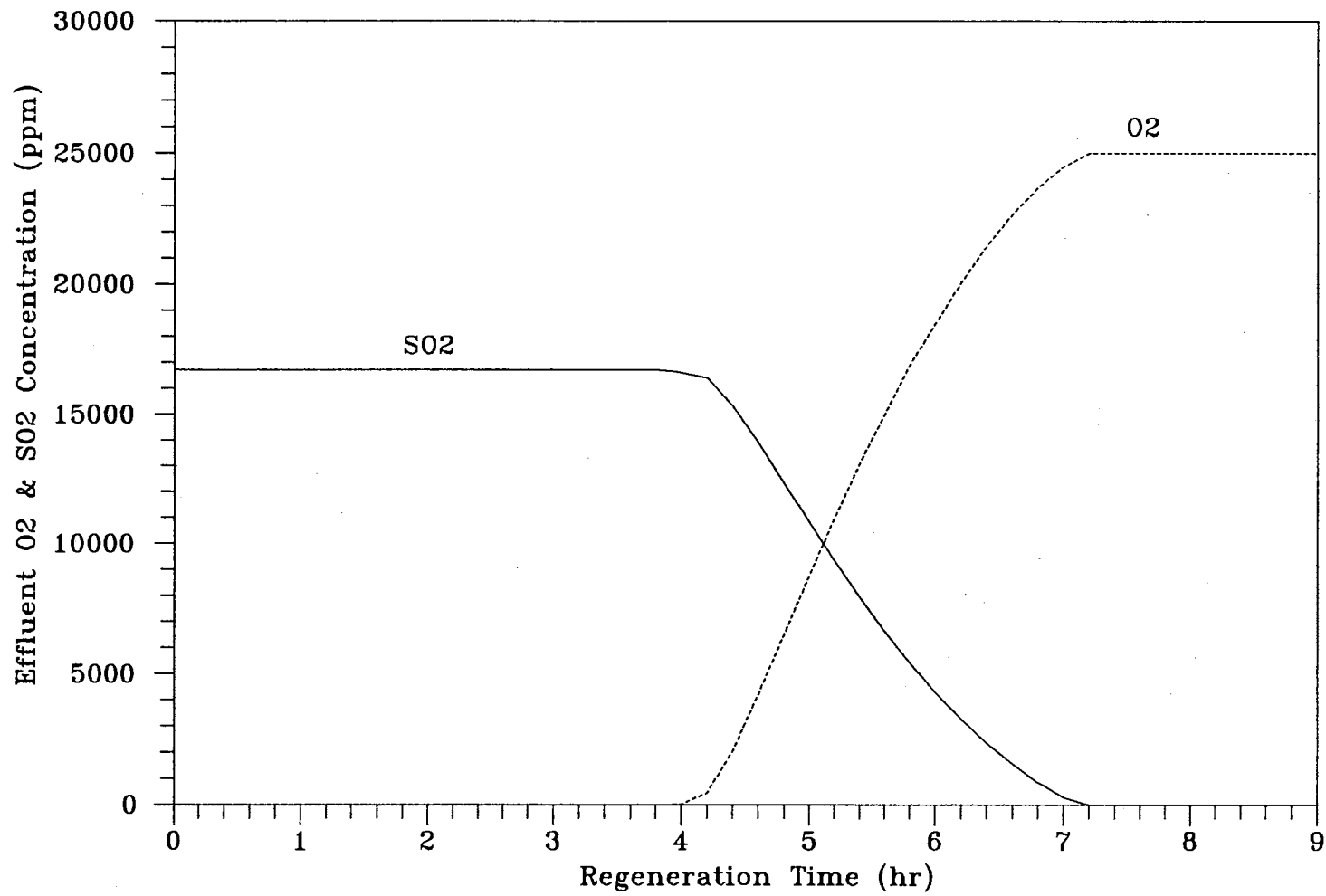


Figure 27. Effluent O₂ & SO₂ Concentration Profiles for Regeneration

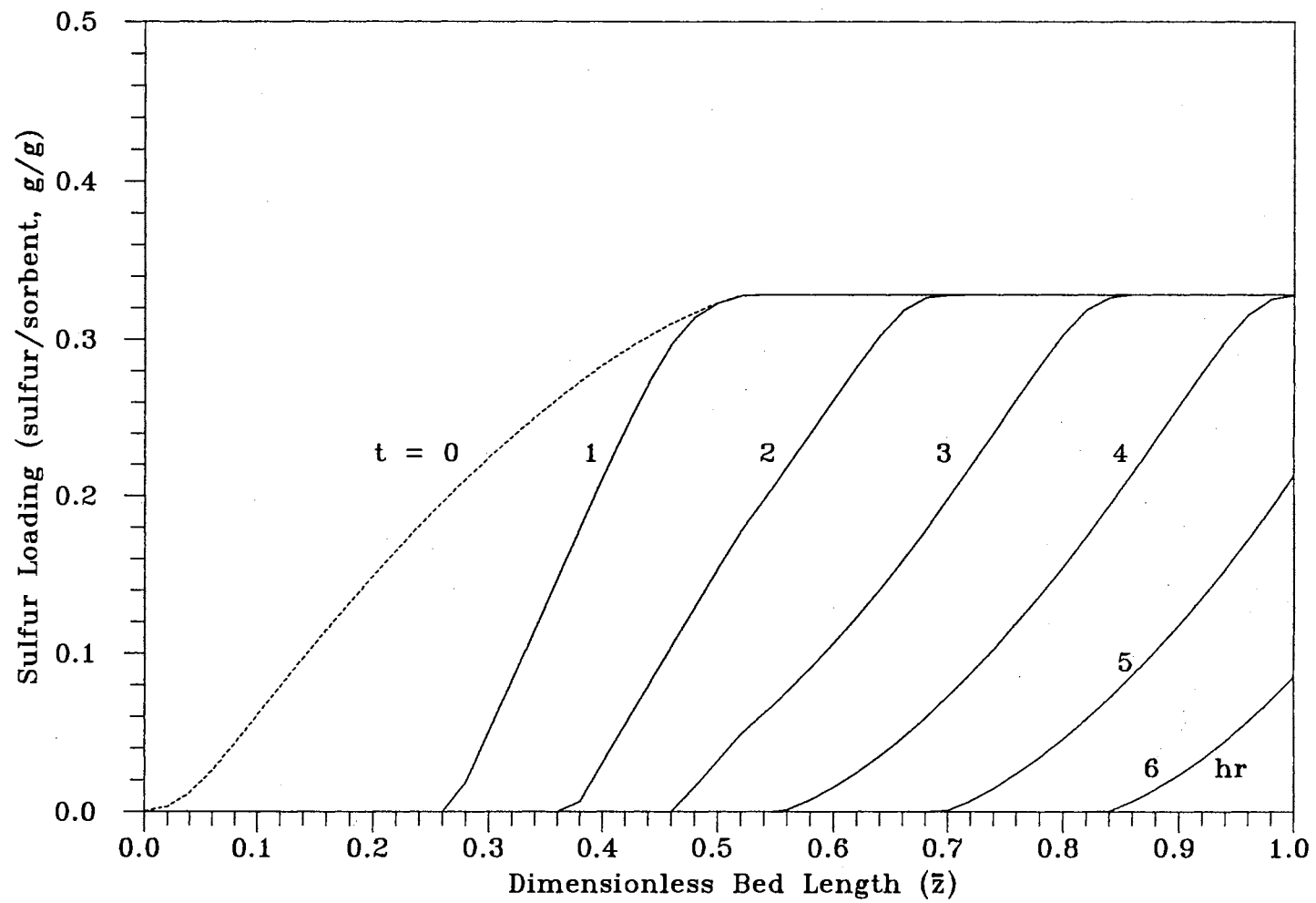


Figure 28. Sulfur Loading Profiles for Regeneration

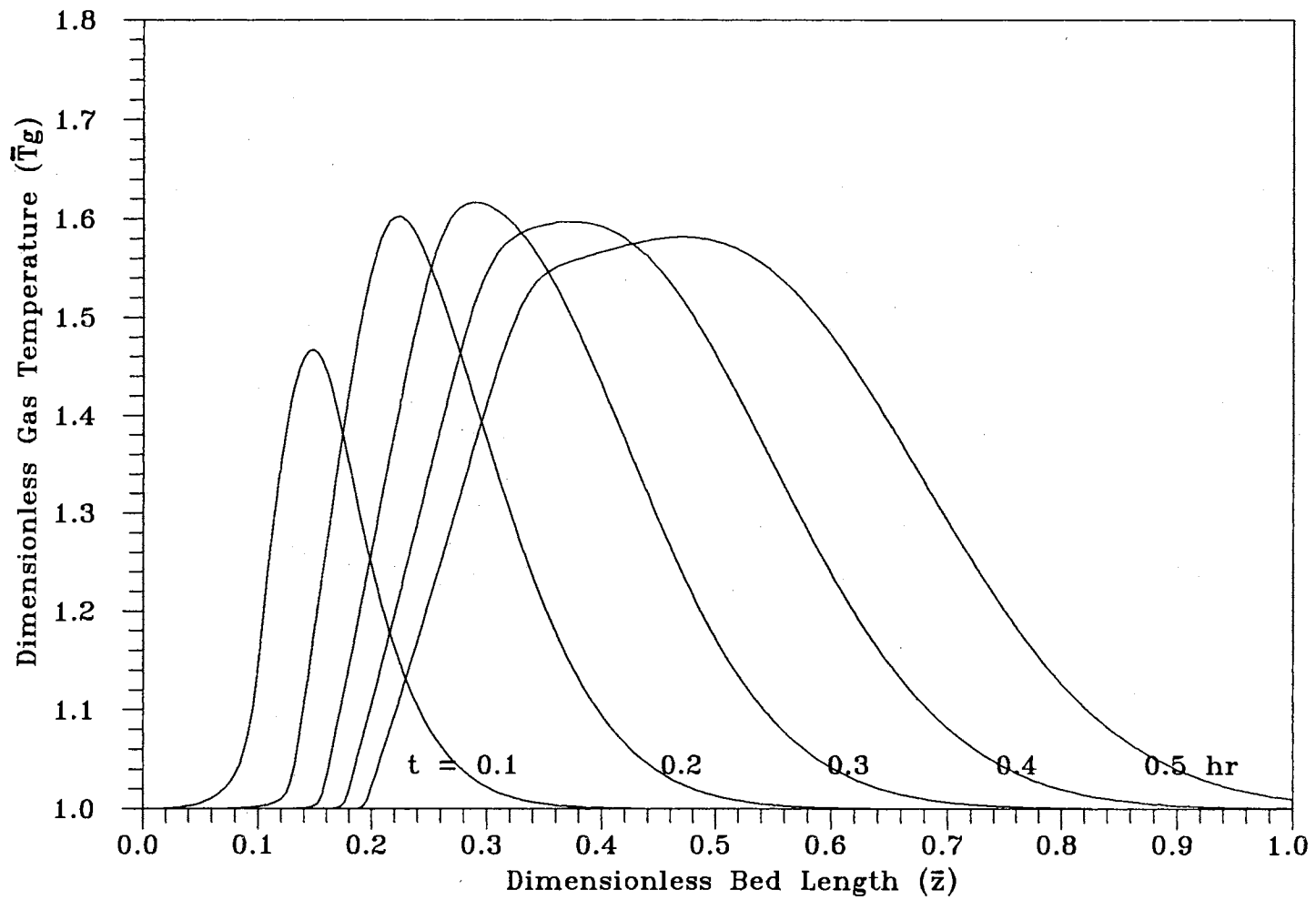


Figure 29. Dimensionless Gas Temperature Profiles for Regeneration

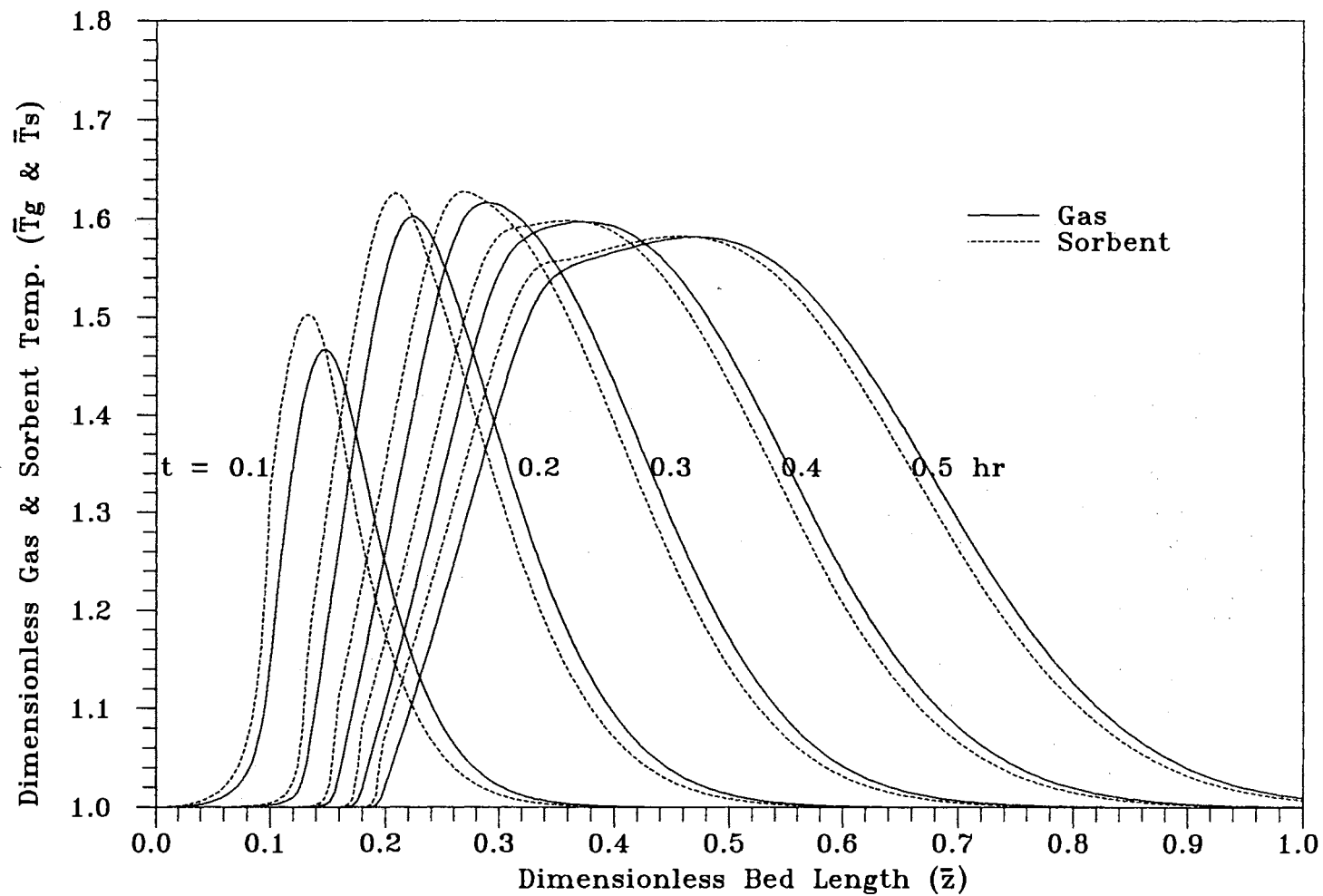


Figure 30. Dimensionless Gas & Sorbent Temperature Profiles for Regeneration

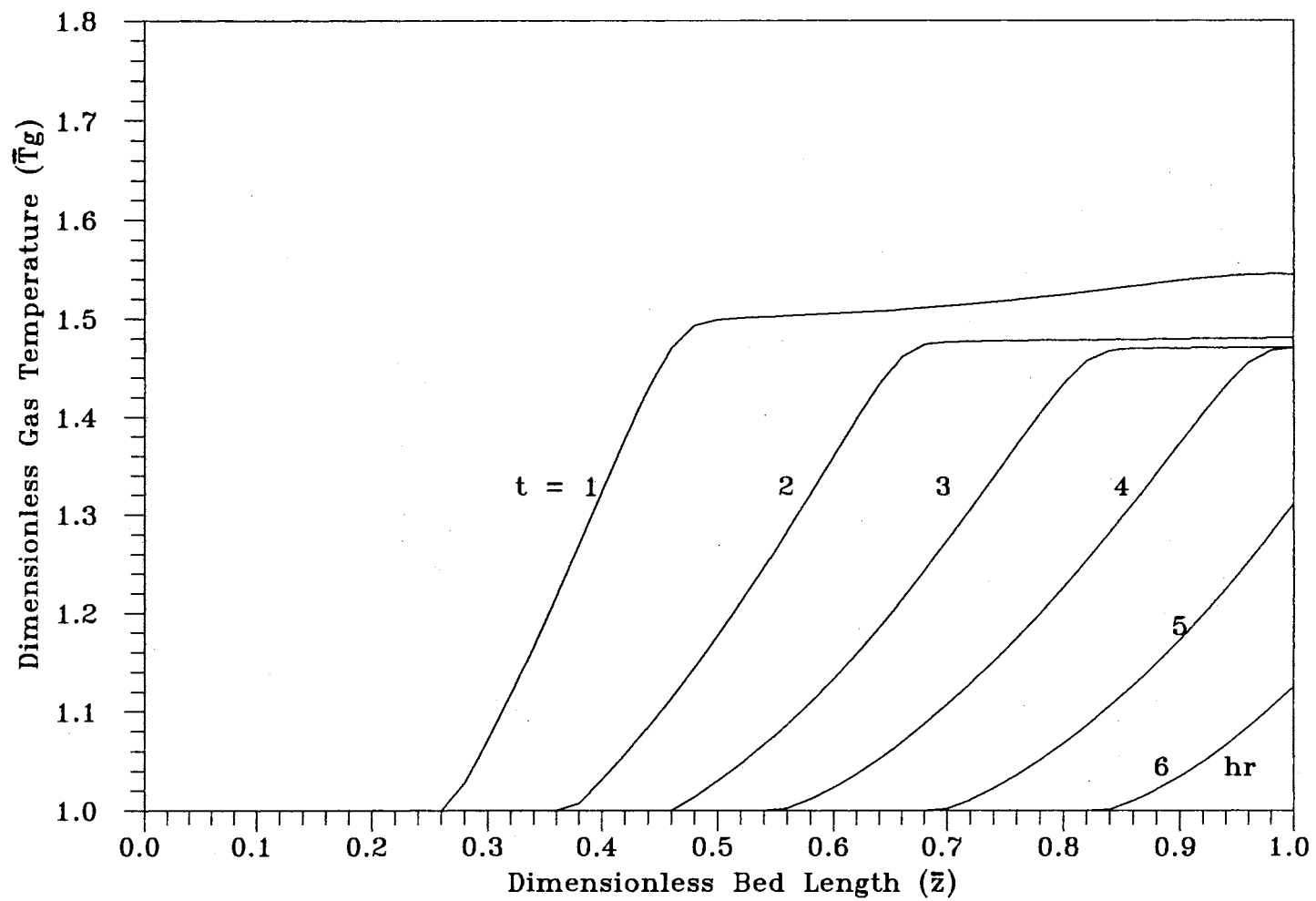


Figure 31. Dimensionless Gas Temperature Profiles
for Regeneration (from 1 to 6 hr)

the sorbents in Figure 32.

Figure 33 shows dimensionless gas temperature profiles as a function of regeneration time at different fixed-bed positions (in the 0 to 0.5 hr time span). The same simulation results shown in this figure were differently presented (i.e., as a function of dimensionless bed length at different times) in Figure 29.

Figure 34 shows dimensionless gas and sorbent temperature profiles as a function of regeneration time at different bed positions (i.e., at $z = 0.1, 0.2, 0.3, 0.5$ and 0.7). This figure is a different version of Figure 30. Figure 35 and 36 are also different versions of Figure 31 and 32, respectively. These figures represent the unsteady state nature of temperature profiles in the fixed-bed.

In the following paragraphs, effects of various parameters on the regeneration sulfur loading and the regeneration gas temperature are discussed.

The effect of superficial gas velocity on the sulfur loading for regeneration is presented in Figure 37. With all other conditions remaining the same, an increase in the superficial gas velocity shows faster regeneration in the regenerator. Higher superficial gas velocity induces the regeneration reaction in a broader range of the regenerator. Thus, strong effect of the superficial gas velocity on the sulfur loading is shown in this figure (at $t = 1$ hr as an example).

The effect of inlet O_2 concentration on the sulfur loading for regeneration is shown in Figure 38. This effect is explained at $t = 1$ hr, as an example. When a higher O_2 inlet concentration was used for regeneration, the less the amount of remaining ZnS was predicted in the regenerator. This means a faster regeneration with a higher reactant concentration.

The effect of inlet gas temperature on the sulfur loading for regeneration is shown in Figure 39. Almost no influence of the inlet gas temperature on the sulfur loading is present in this figure. Remaining sulfur in the regenerator at $t = 1$ hr is shown when inlet gas temperatures are 550, 700 and 850 K, respectively.

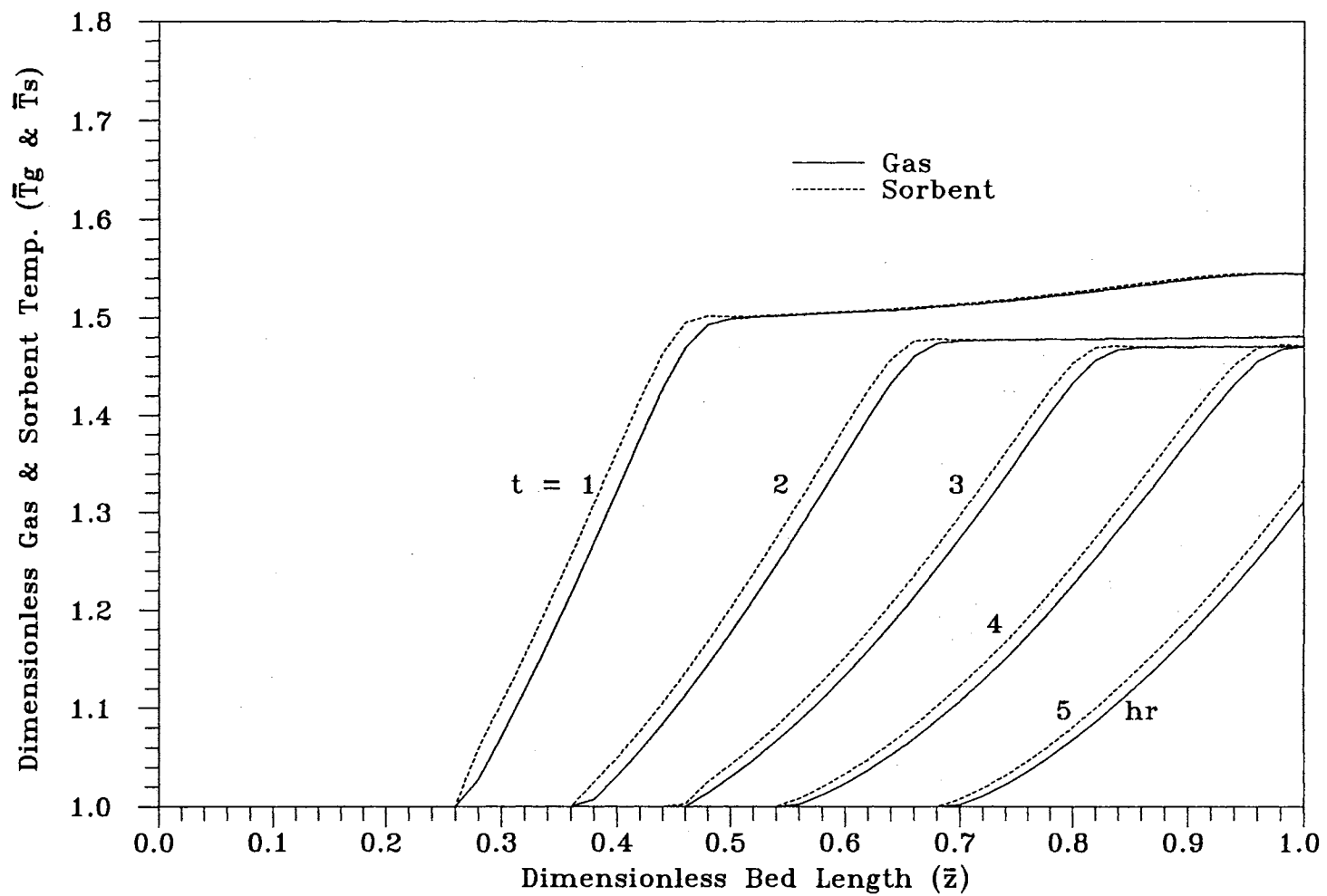


Figure 32. Dimensionless Gas & Sorbent Temperature Profiles for Regeneration (from 1 to 5 hr)

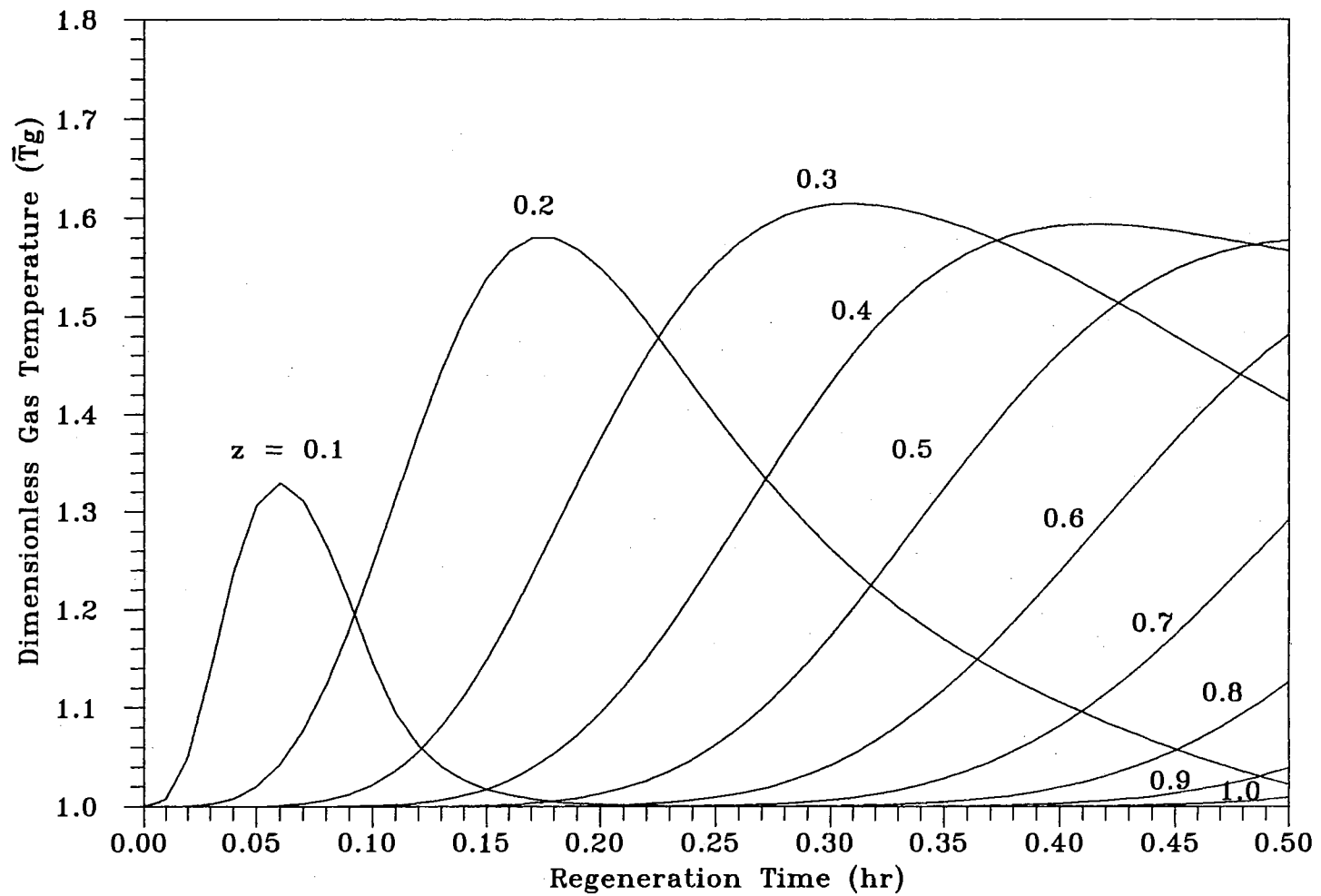


Figure 33. Dimensionless Gas Temperature Profiles for Regeneration at Different Bed Positions

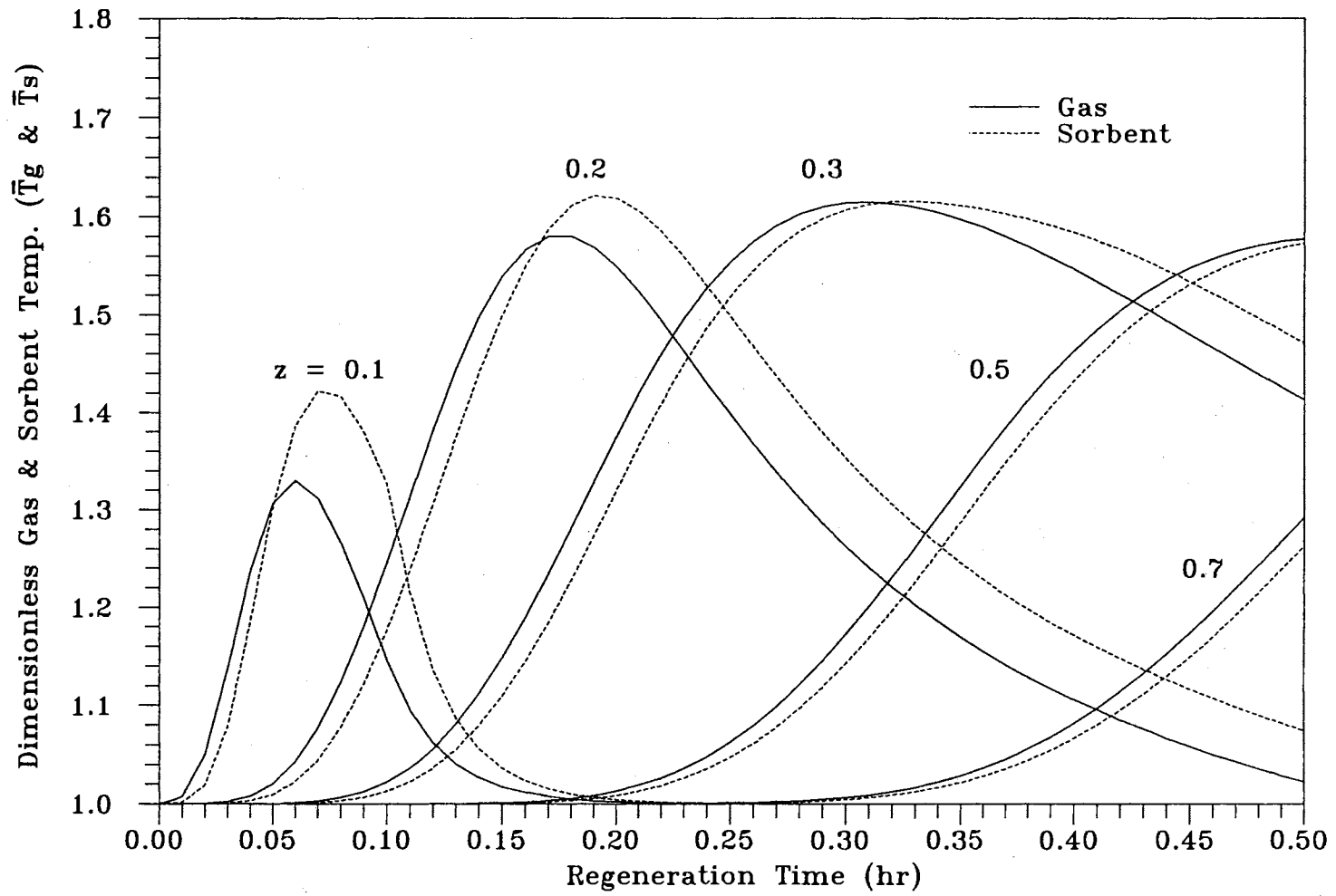


Figure 34. Dimensionless Gas & Sorbent Temperature Profiles for Regeneration at Different Bed Positions

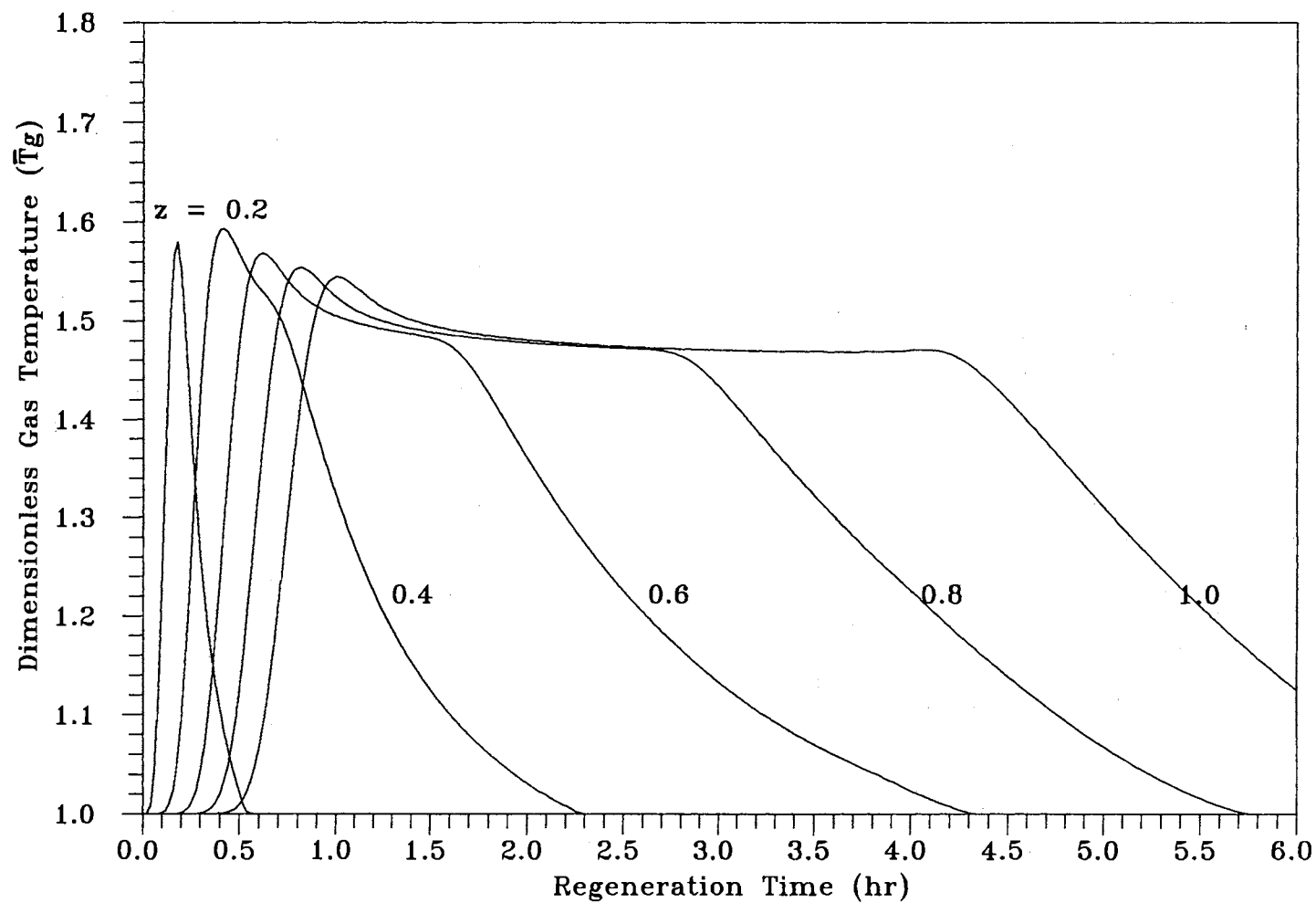


Figure 35. Dimensionless Gas Temperature Profiles for Regeneration at Different Bed Positions (II)

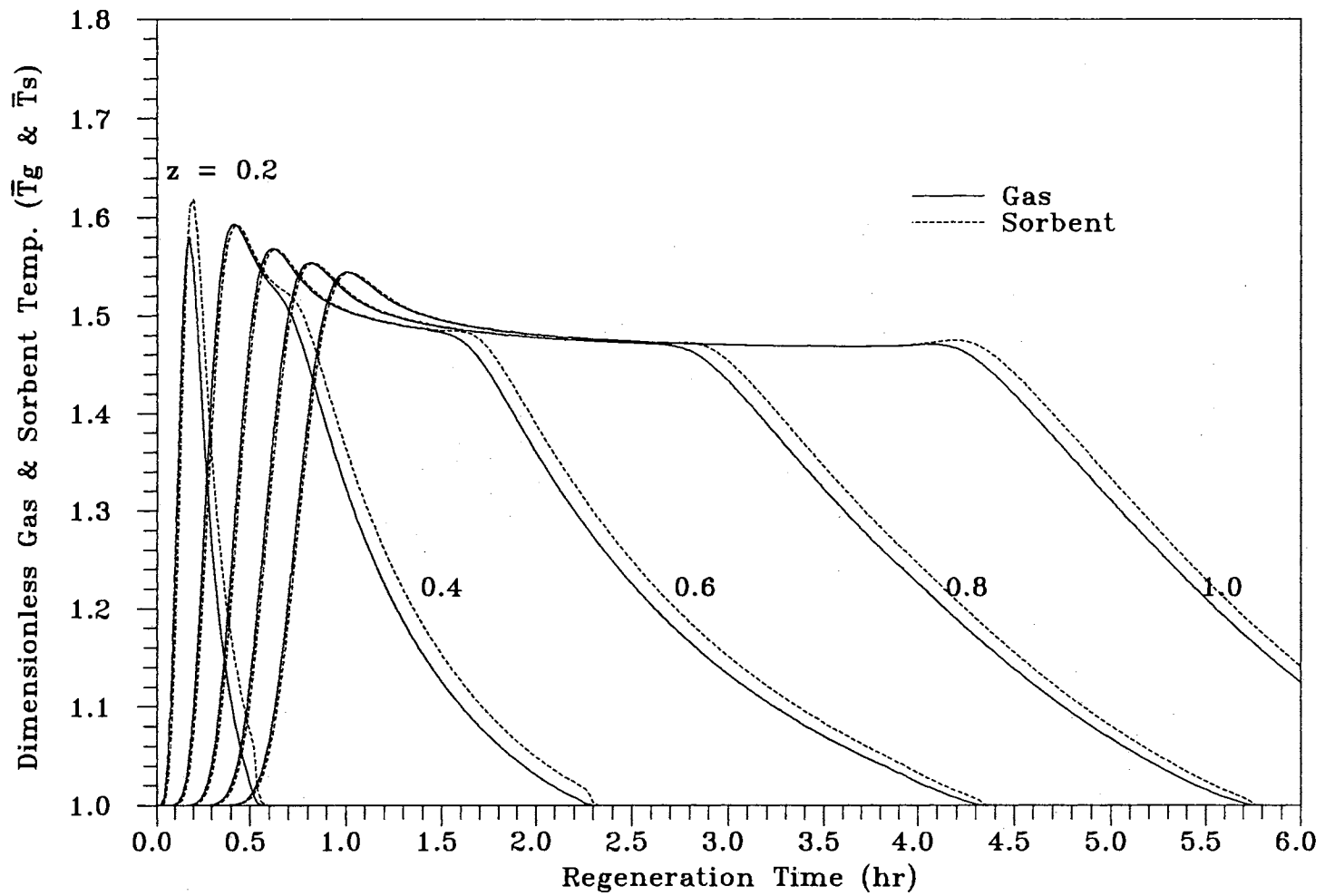


Figure 36. Dimensionless Gas & Sorbent Temperature Profiles for Regeneration at Different Bed Positions (II)

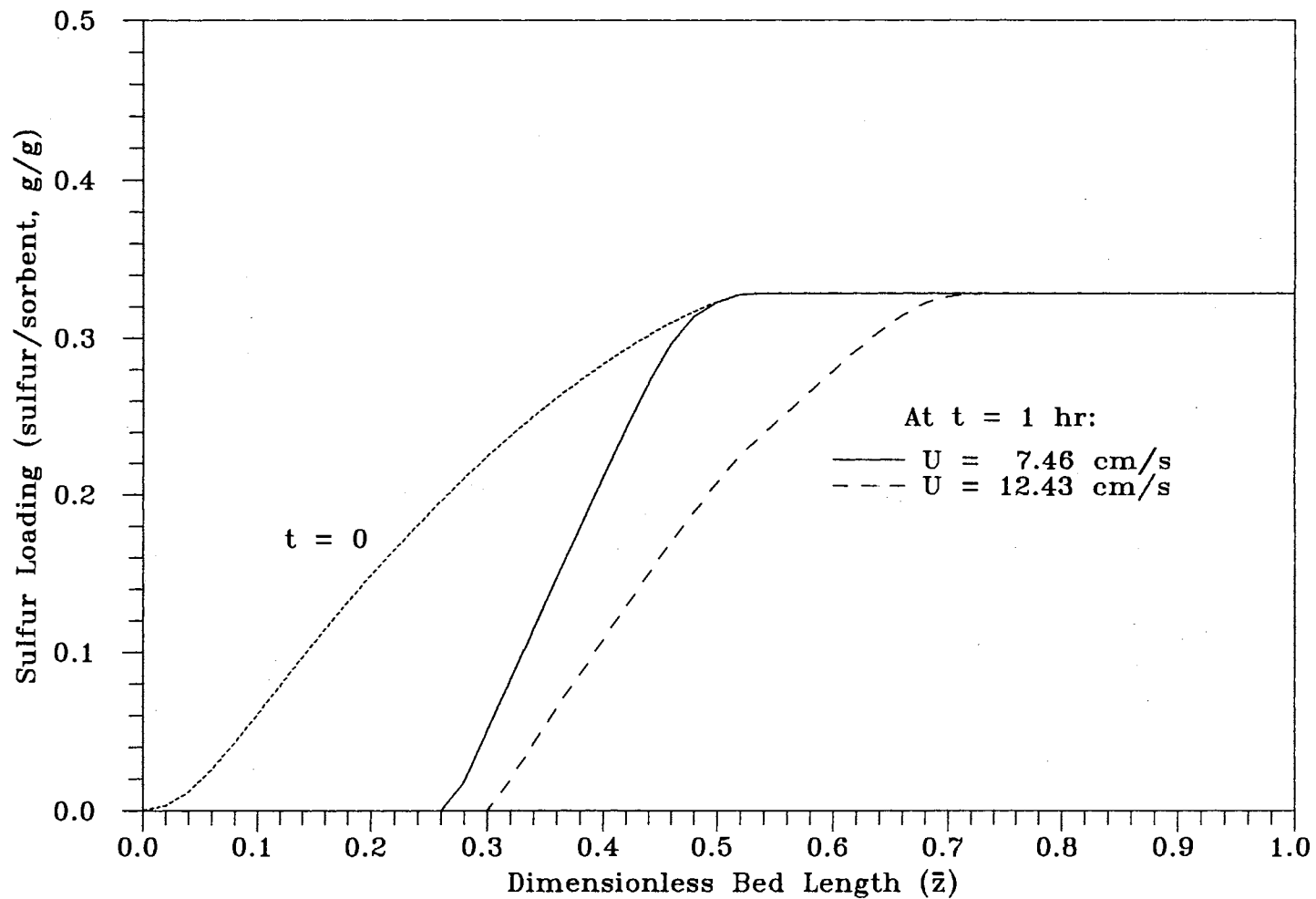


Figure 37. Effect of Superficial Gas Velocity on Sulfur Loading for Regeneration

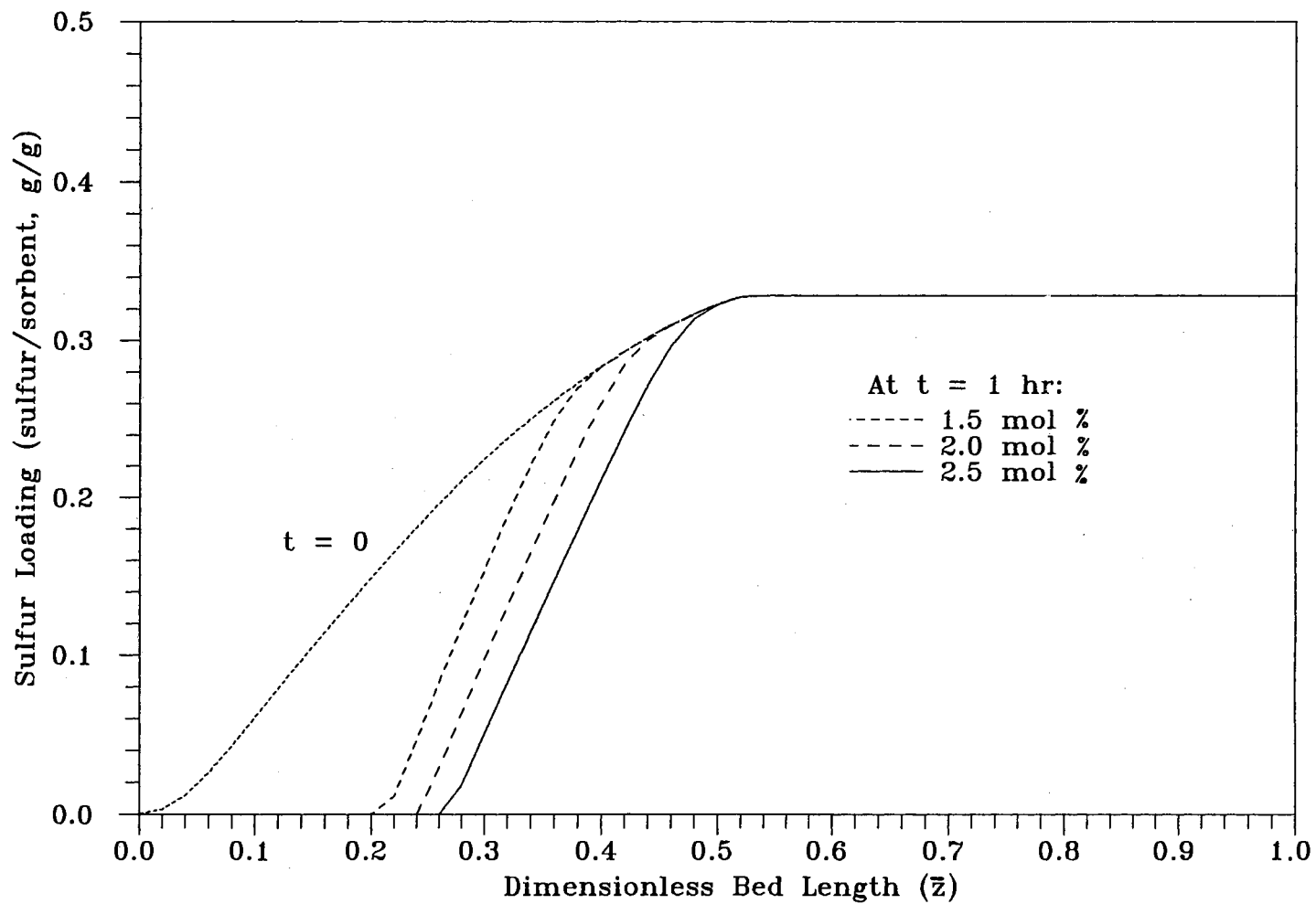


Figure 38. Effect of Inlet O_2 Concentration on Sulfur Loading for Regeneration

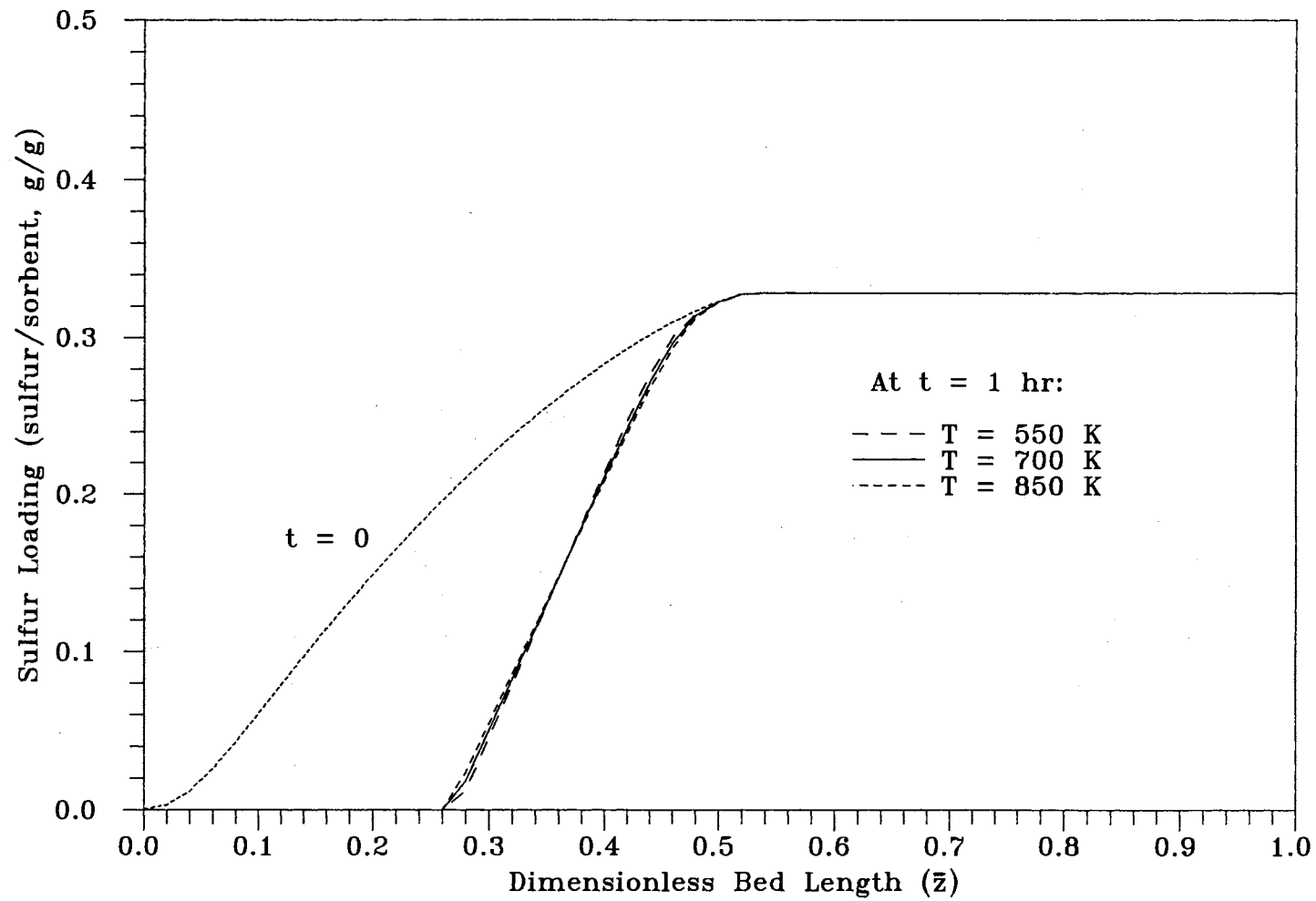


Figure 39. Effect of Inlet Gas Temperature on Sulfur Loading for Regeneration

The effect of inlet O_2 concentration on the gas temperature in the regenerator is shown in Figure 40. A very sensitive effect of the inlet O_2 concentration on the gas temperature rise is observed at $t = 0.4$ hr, as an example. When the inlet O_2 concentration was reduced, the gas temperature rise was drastically decreased. This phenomena is also true for the sorbents (not shown in this figure). The controlling of the inlet O_2 concentration is very important in safe operation of the regenerator. A severe temperature increase may induce sintering of the sorbents.

The effect of superficial gas velocity on the gas temperature in the regenerator is shown in Figure 41. The higher superficial gas velocity results in the lower gas temperature increase and shows the spread of the gas temperature profile in a broader range of the regenerator.

Pilot Plant Scale Tail gas Clean-up System

In this section, simulation results for the pilot plant scale system are briefly discussed. Numerical values of model parameters for the sulfidation and regeneration cases were shown in Chapter VI (i.e., in Table VII and Table VIII, respectively). General features of the pilot plant scale system are similar to those of the lab-scale system.

Results from the Sulfidation Simulation

Figure 42 shows a predicted H_2S breakthrough curve for the complete sulfidation of fresh ZnO/Al_2O_3 sorbents in the adiabatic fixed-bed reactor. Obviously, the operation of a sulfidation reactor for tail gas clean-up is stopped at (or just before) a preset breakthrough concentration. At this time, the sorbents in the reactor are partially sulfided and the effluent H_2S concentration from the reactor should be lower than the limit of the air pollution regulations. In this figure, the computed breakthrough time is 34.9 hr when

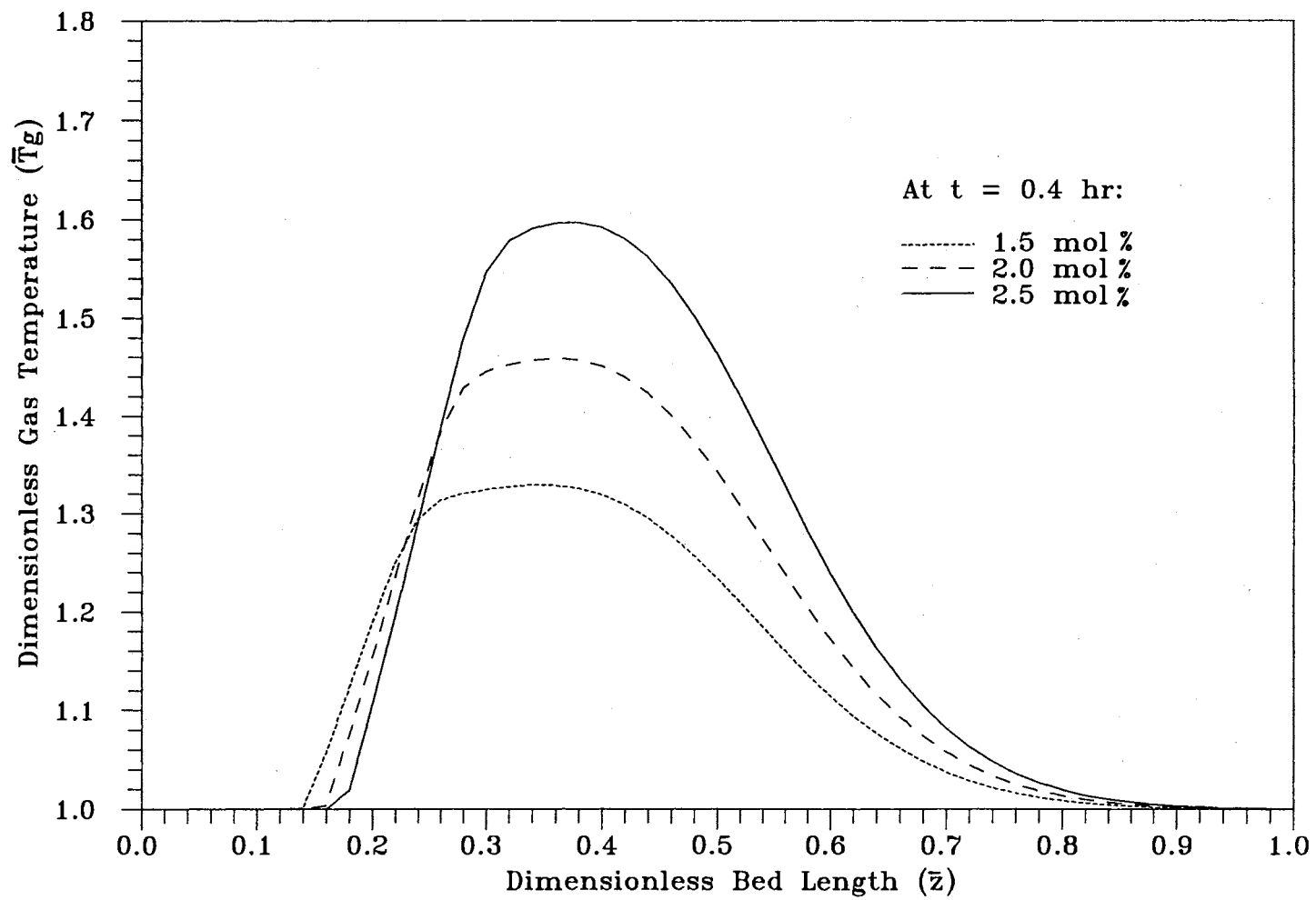


Figure 40. Effect of Inlet O₂ Concentration on Gas Temperature for Regeneration

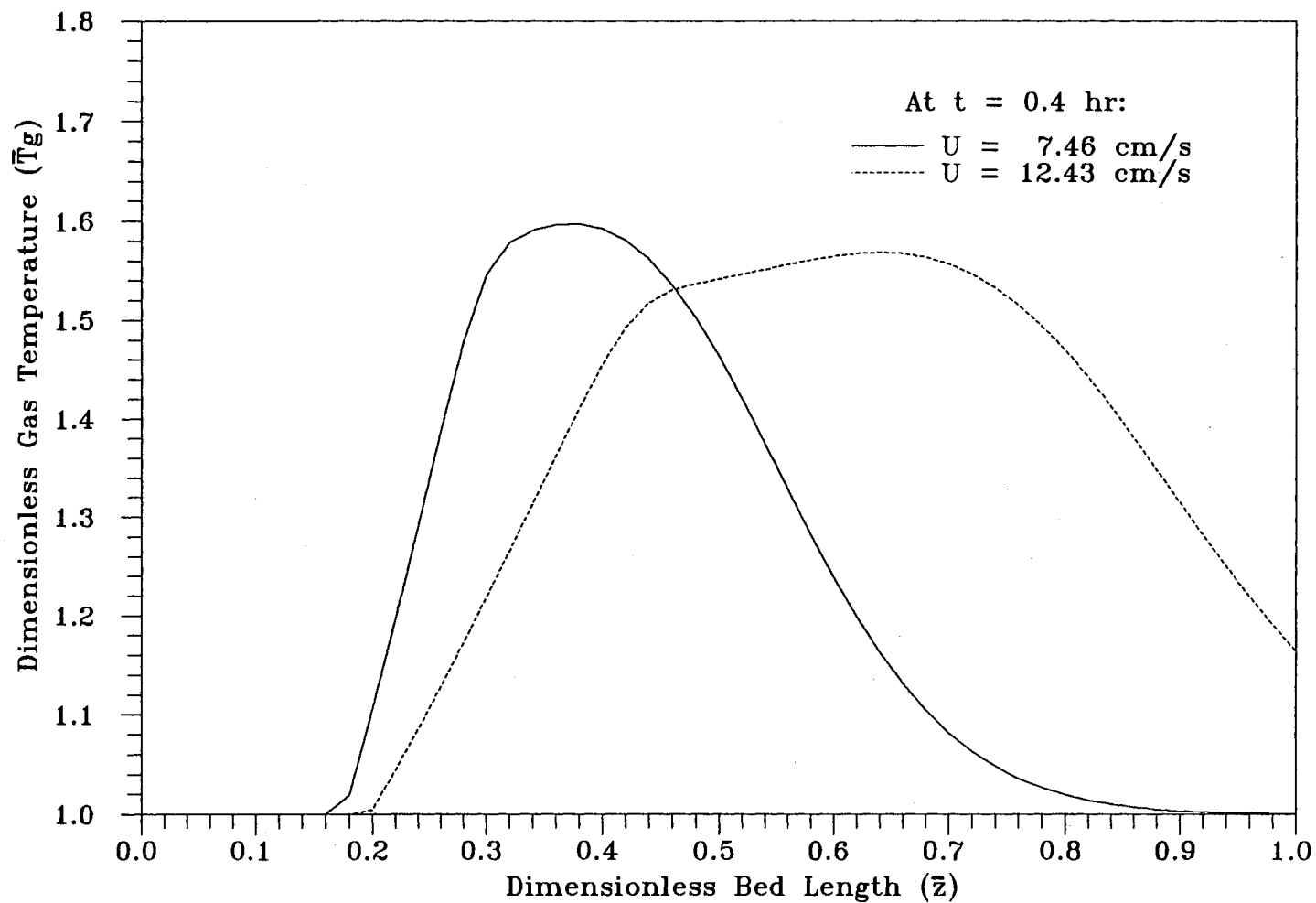


Figure 41. Effect of Superficial Gas Velocity on Gas Temperature for Regeneration

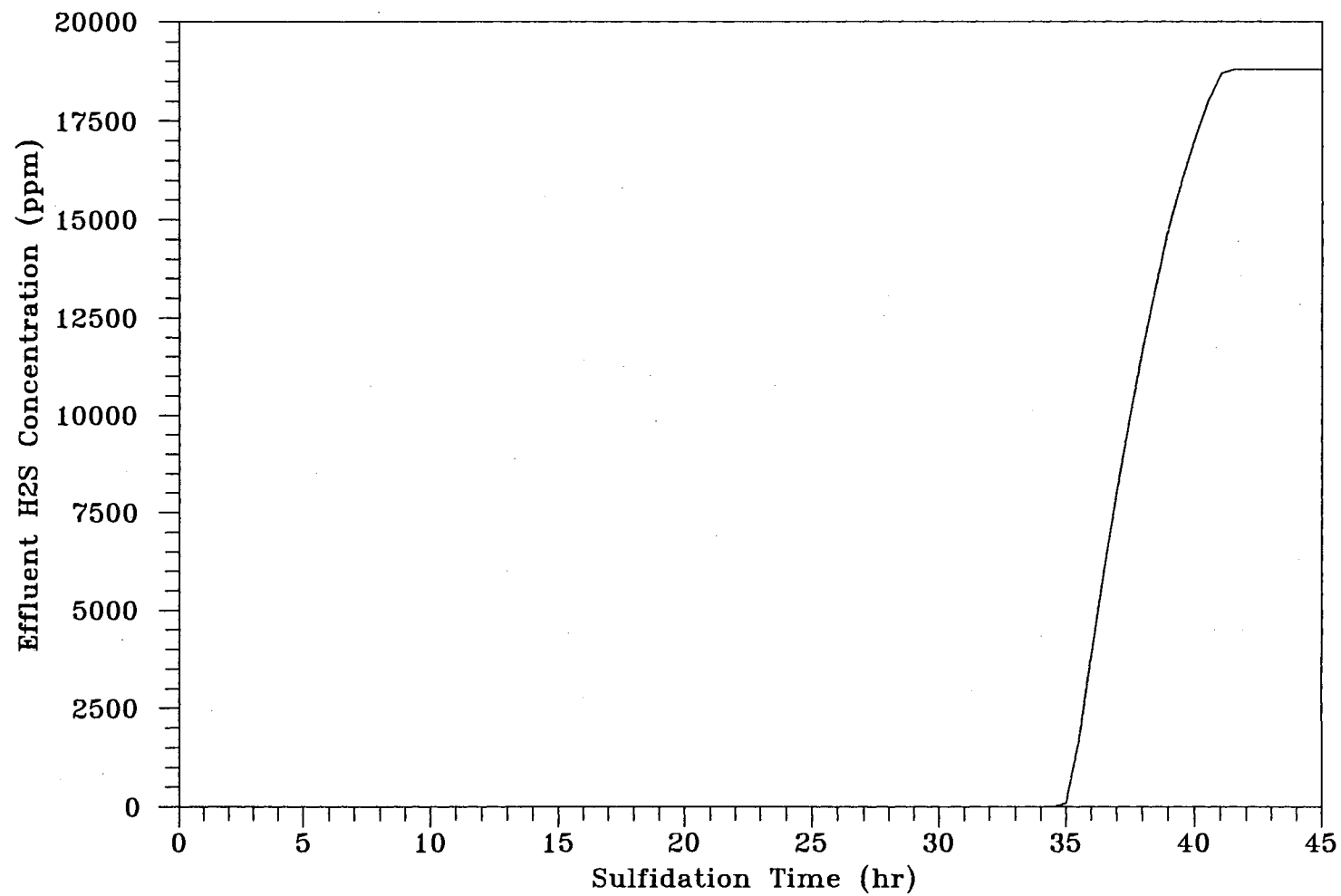


Figure 42. Breakthrough Curve for Sulfidation (pilot plant)

the effluent H_2S concentration is 30 ppmv.

Figure 43 shows dimensionless H_2S concentration profiles in the sulfidation reactor. After about 3 hours, sulfidation reaction fronts with the same pattern start traveling along the fixed-bed reactor. At selected times (i.e., the same times as those of shown in Figure 43), sorbent conversion profiles and sulfur loading profiles are shown in Figure 44 and Figure 45, respectively. In Figure 44, the average sorbent conversion in the reactor at the breakthrough time is 0.9295.

Figure 46 shows dimensionless gas temperature profiles in the reactor at $t = 0.5$, 1.0, 1.5 and 2.0 hr. At these selected times, dimensionless gas and sorbent temperature profiles are compared in Figure 47. Almost no temperature difference between the gas and the sorbent is predicted. At $t = 2$ hr, the inlet region of the reactor is still under the sulfidation reaction.

Figure 48 shows dimensionless gas temperature profiles in the reactor at selected times (at $t = 5, 10, 15, 20, 25, 30$, and 35 hr). In Figure 49, dimensionless gas and sorbent temperature profiles are compared and no appreciable change between them are observed. After about 5 hr, the peak temperature of the gas and sorbent approaches an asymptotic value.

Results from the Regeneration Simulation.

Figure 50 shows the O_2 breakthrough curve in the regenerator. Corresponding effluent SO_2 concentration versus regeneration time is presented in Figure 51. When the effluent SO_2 concentration reaches to 1000 ppmv, the operation of the regenerator is stopped. Corresponding regeneration time is 25.37 hr. Effluent O_2 and SO_2 concentrations versus regeneration time are shown in Figure 52.

Figure 53 shows the initial sulfur loading profile at the time of starting the regeneration. The sulfur loading profiles with the progress of regeneration are shown

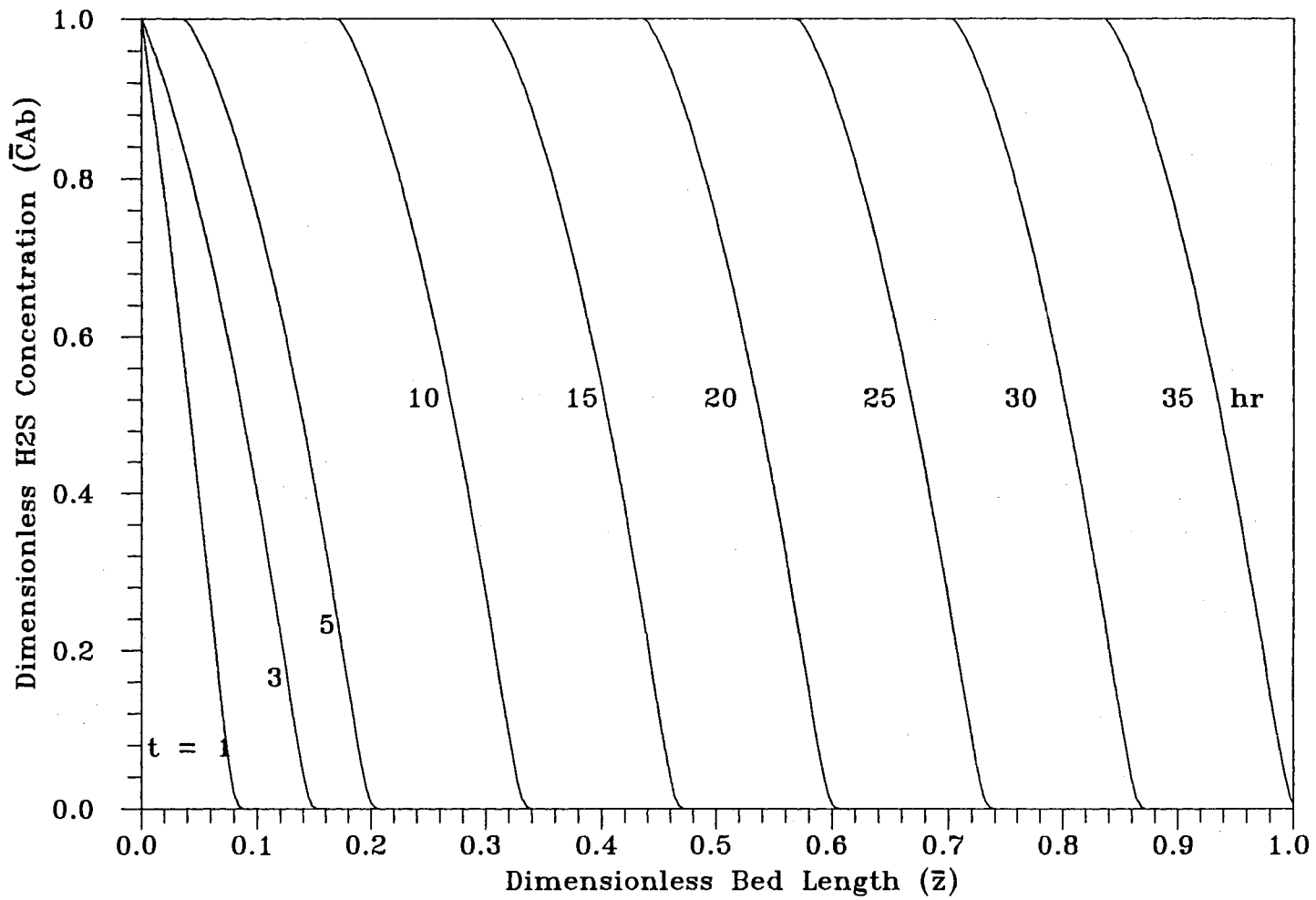


Figure 43. Dimensionless H₂S Concentration Profiles for Sulfidation (pilot plant)

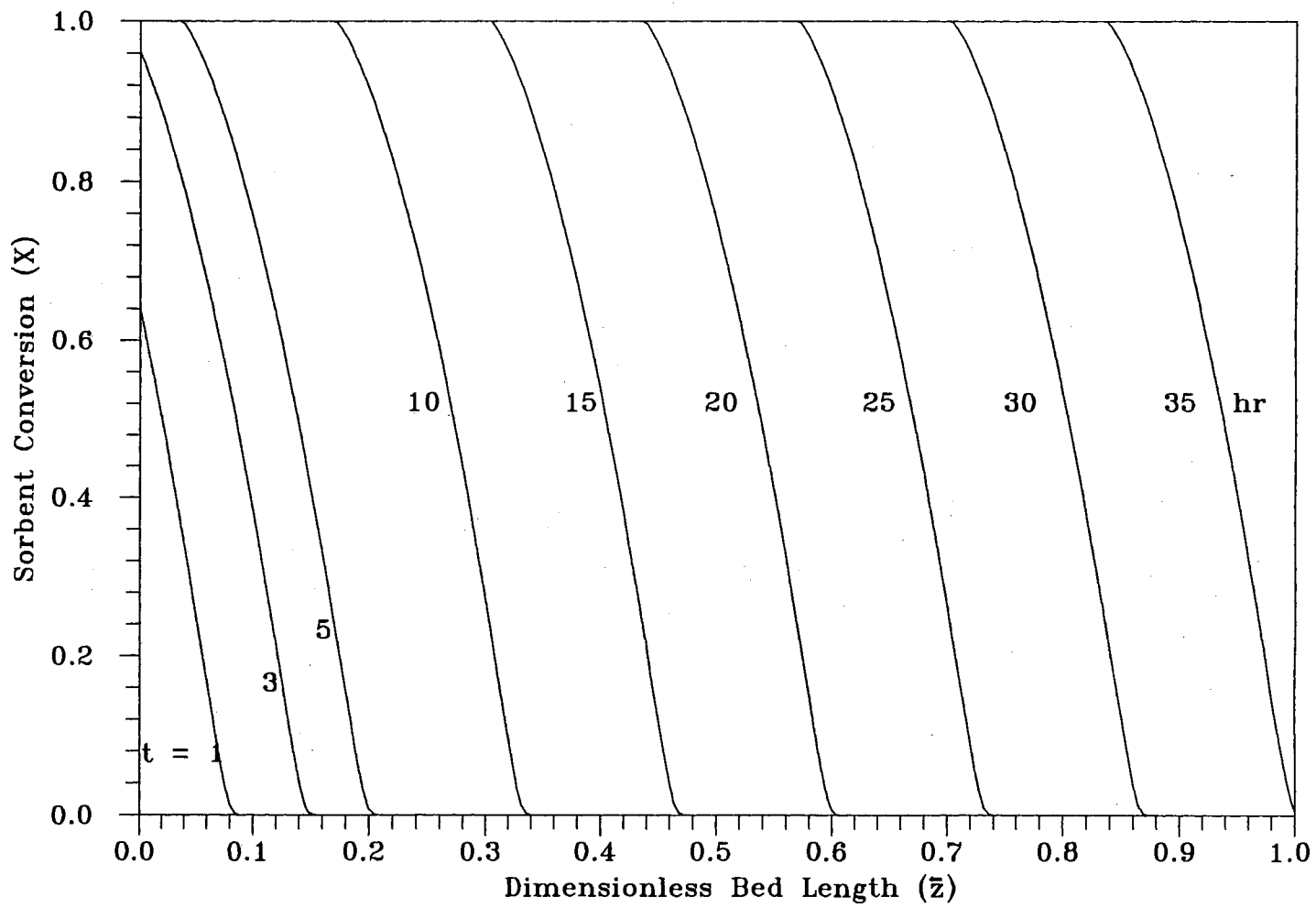


Figure 44. Sorbent Conversion Profiles for Sulfidation (pilot plant)

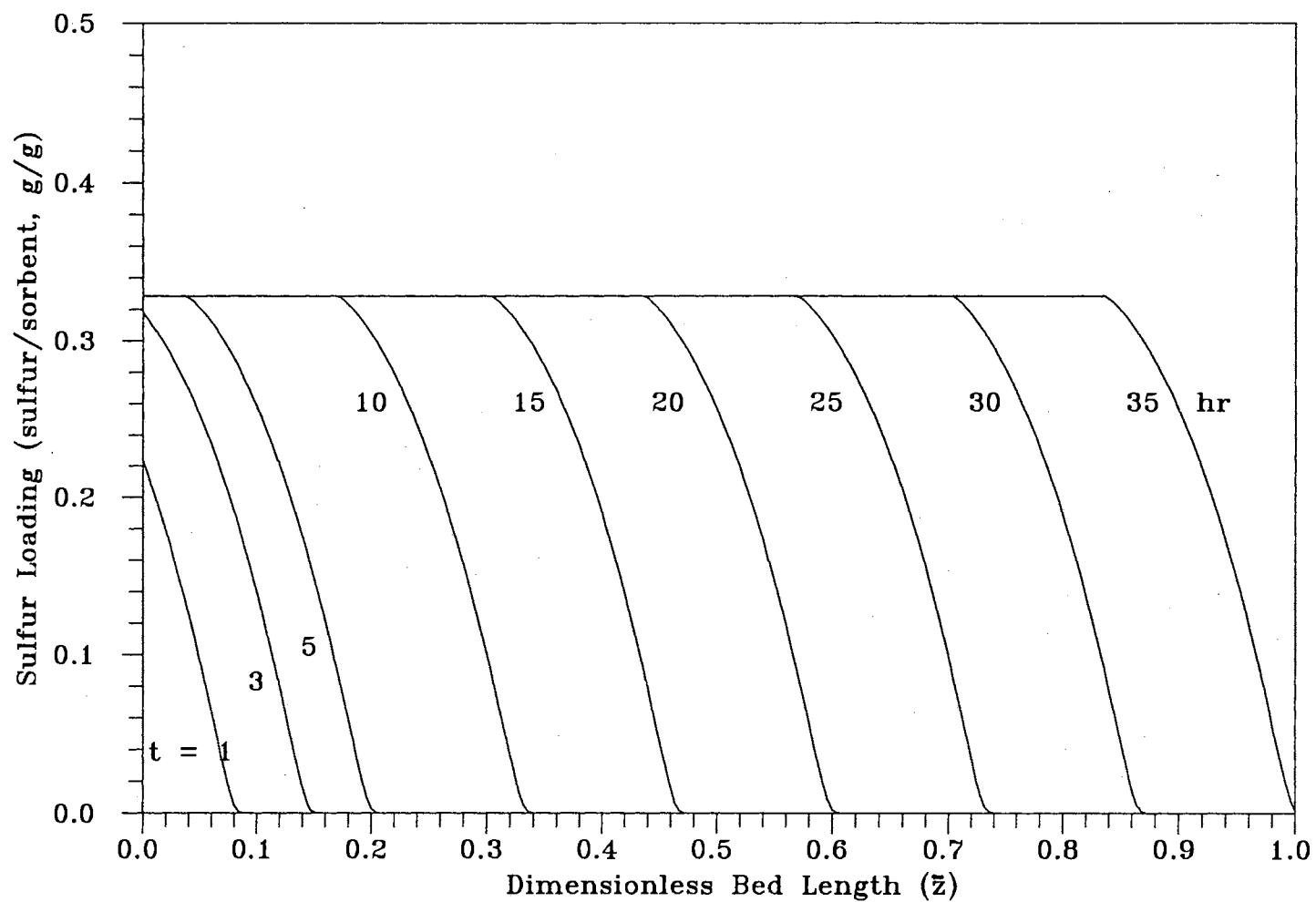


Figure 45. Sulfur Loading Profiles for Sulfidation (pilot plant)

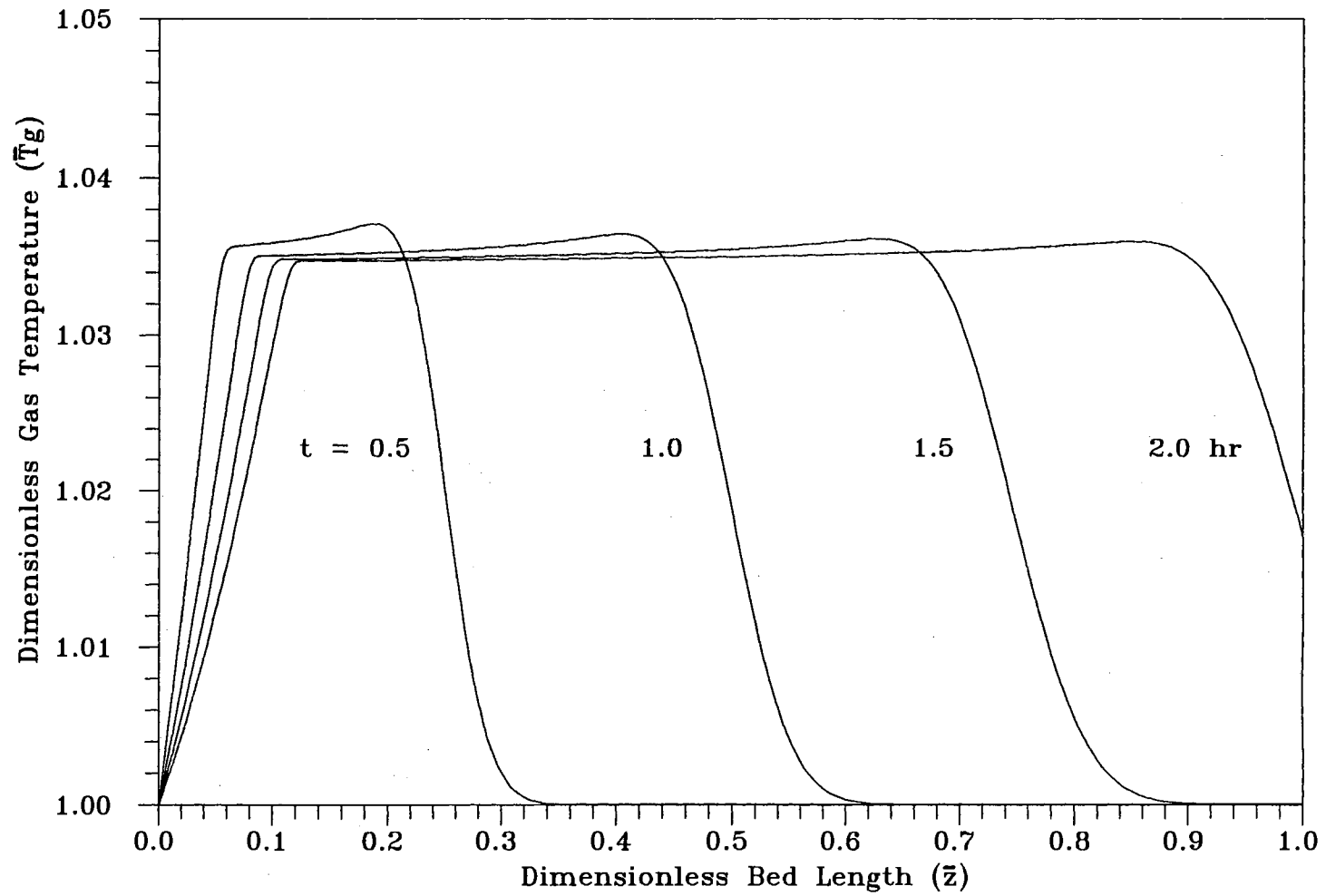


Figure 46. Dimensionless Gas Temperature Profiles for Sulfidation (pilot plant)

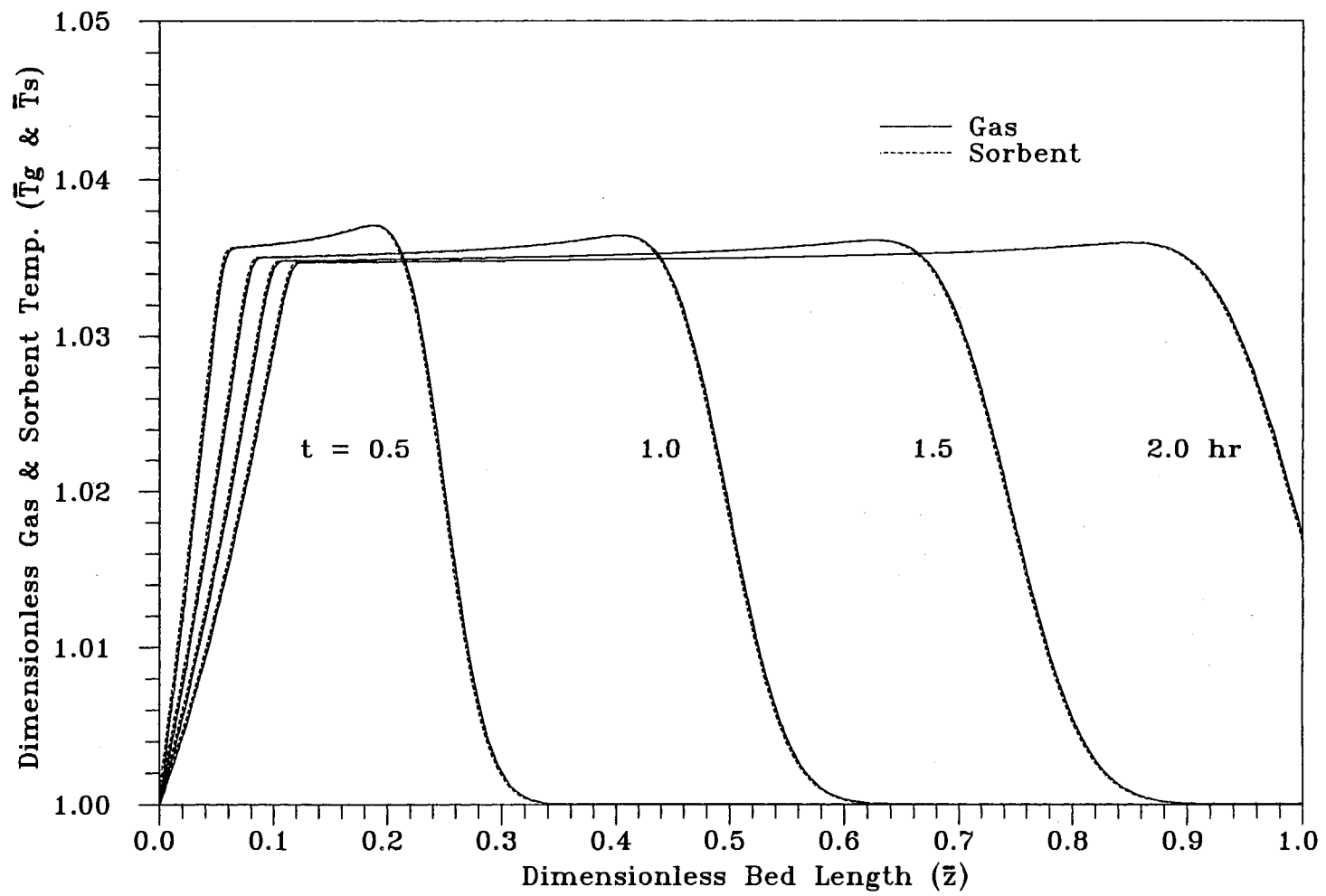


Figure 47. Dimensionless Gas & Sorbent Temperature Profiles for Sulfidation (pilot plant)

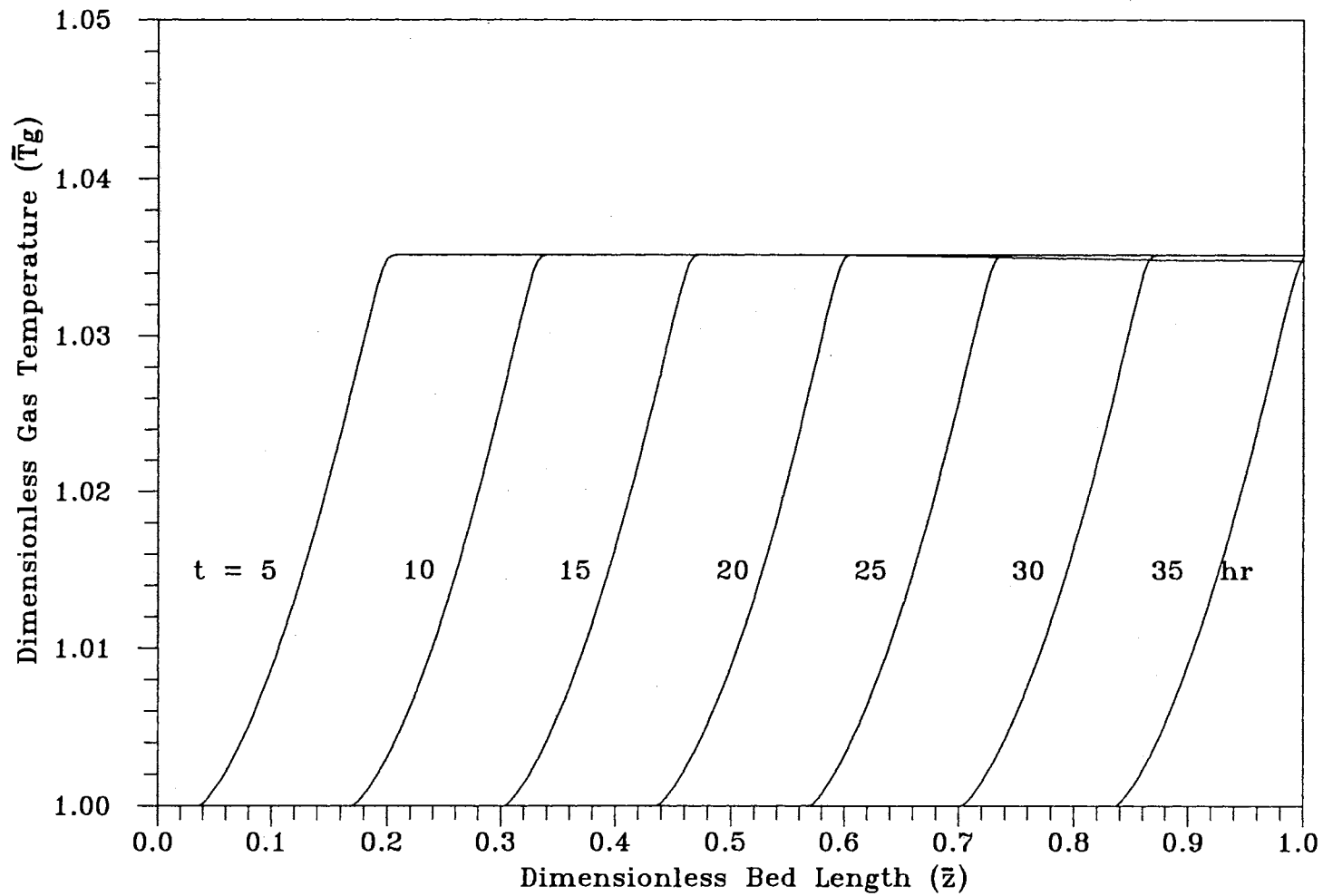


Figure 48. Dimensionless Gas Temperature Profiles for Sulfidation (pilot plant; 5-35 hr)

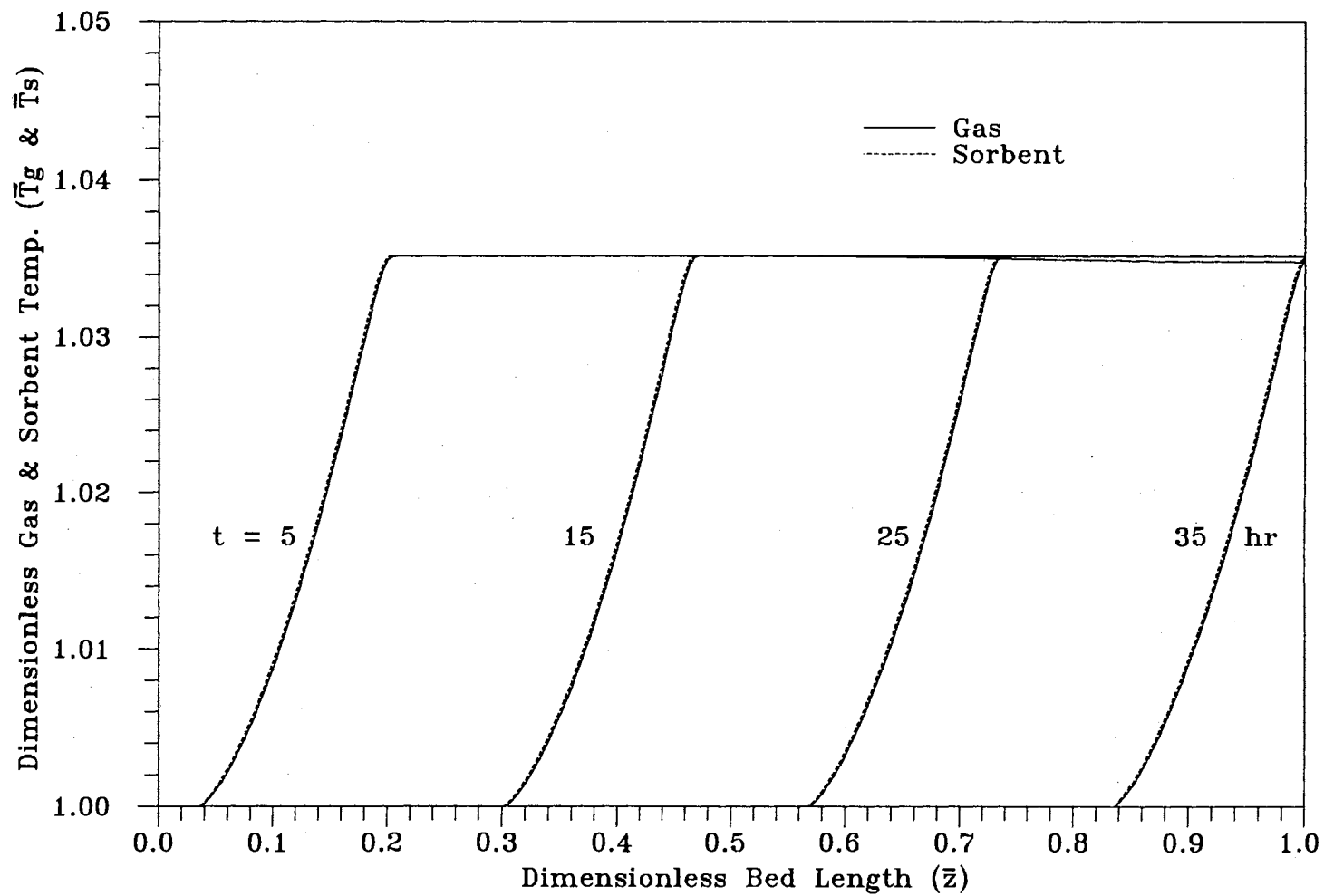


Figure 49. Dimensionless Gas & Sorbent Temperature Profiles for Sulfidation (pilot plant; 5-35 hr)

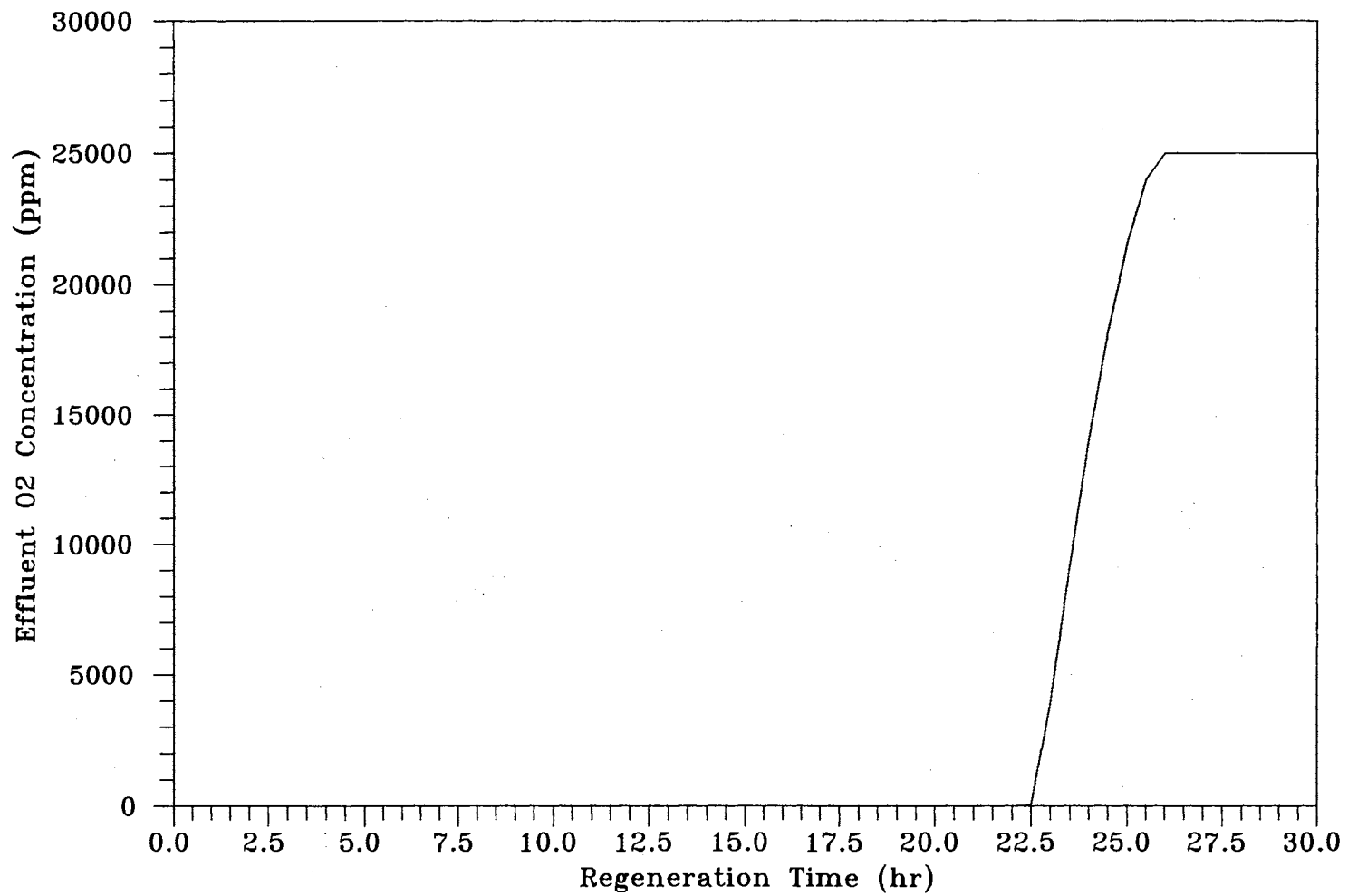


Figure 50. Breakthrough Curve for Regeneration (pilot plant)

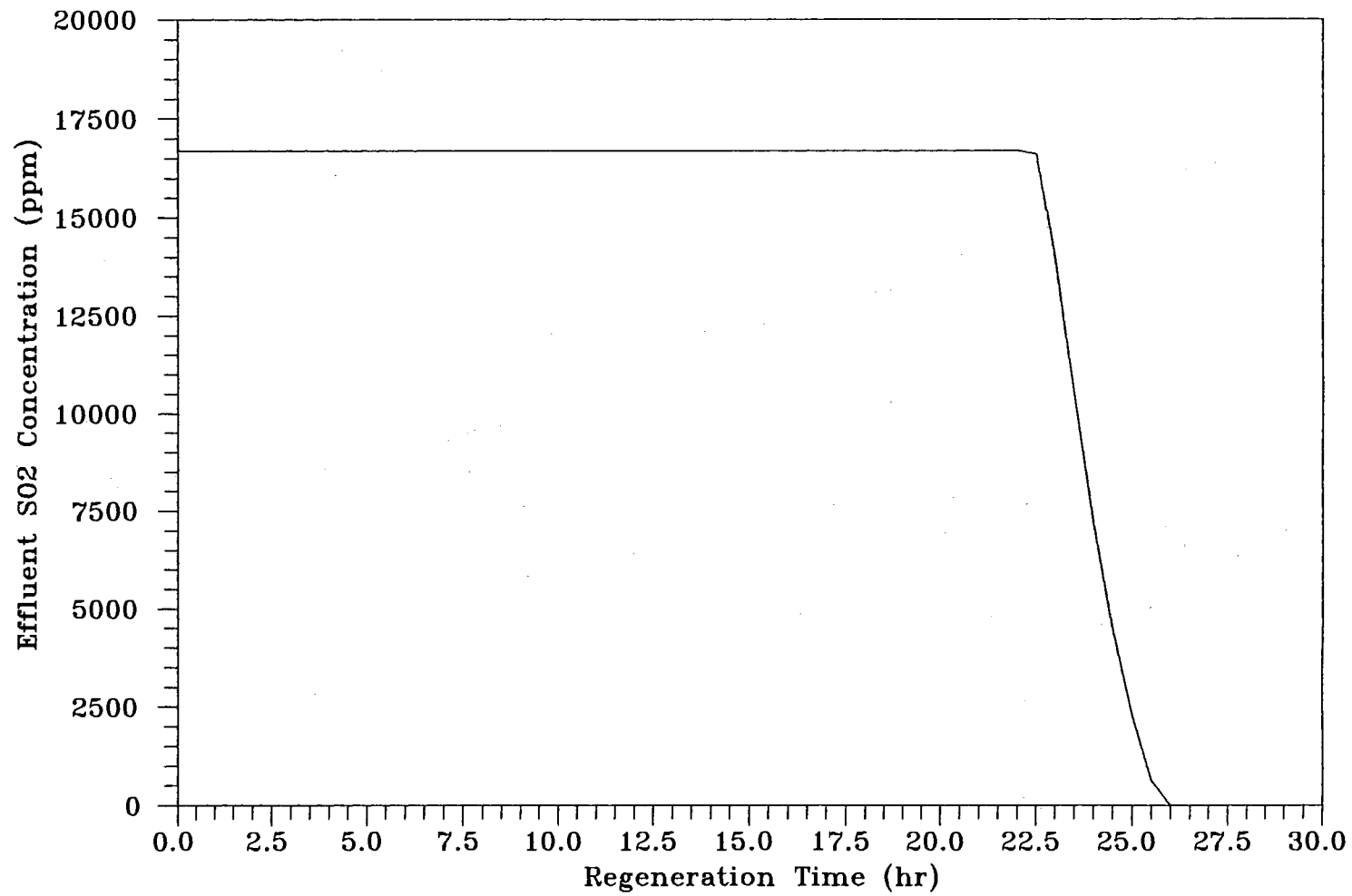


Figure 51. Effluent SO₂ Concentration Profile for Regeneration (pilot plant)

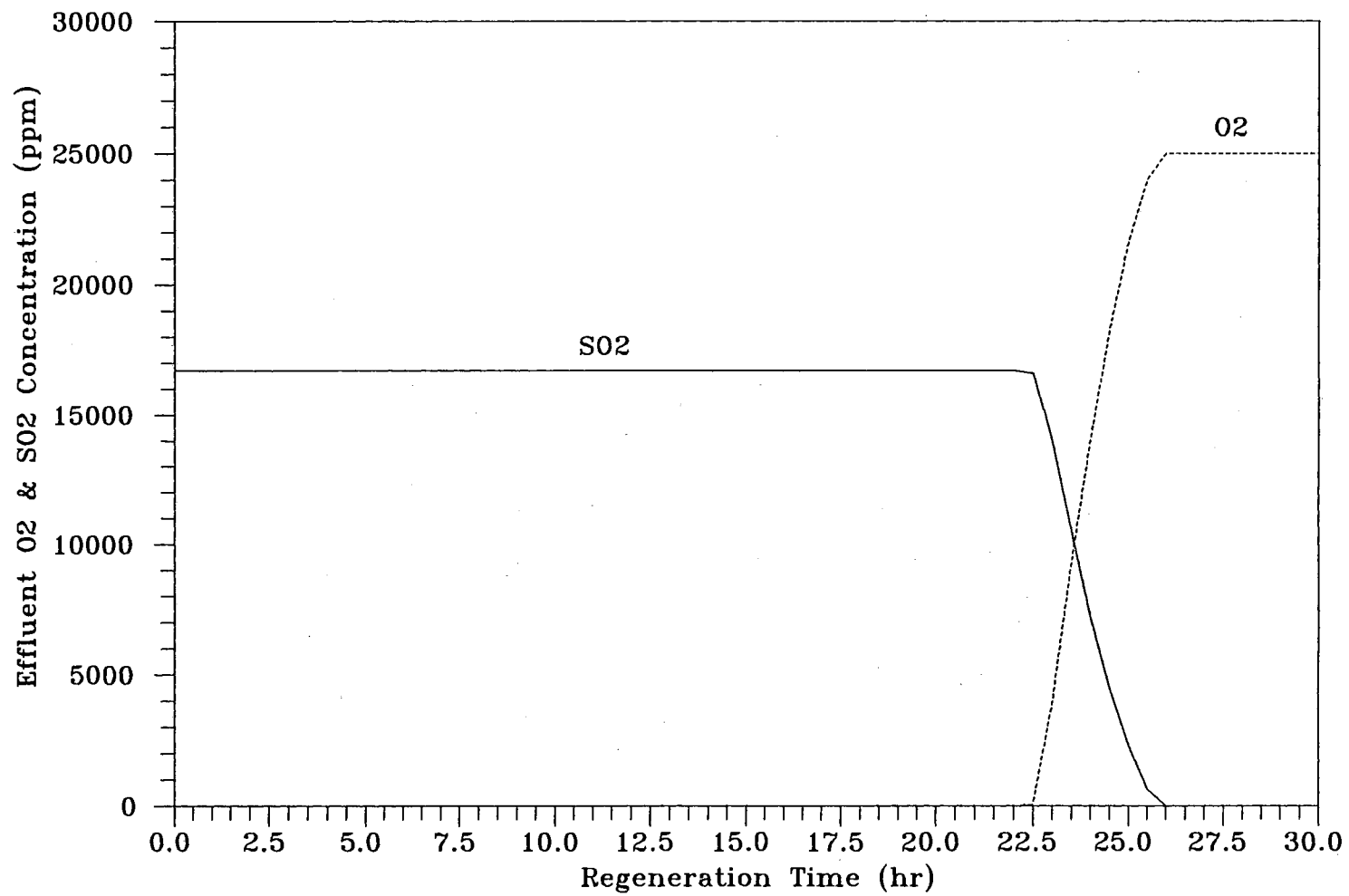


Figure 52. Effluent O₂ & SO₂ Concentration Profiles for Regeneration (pilot plant)

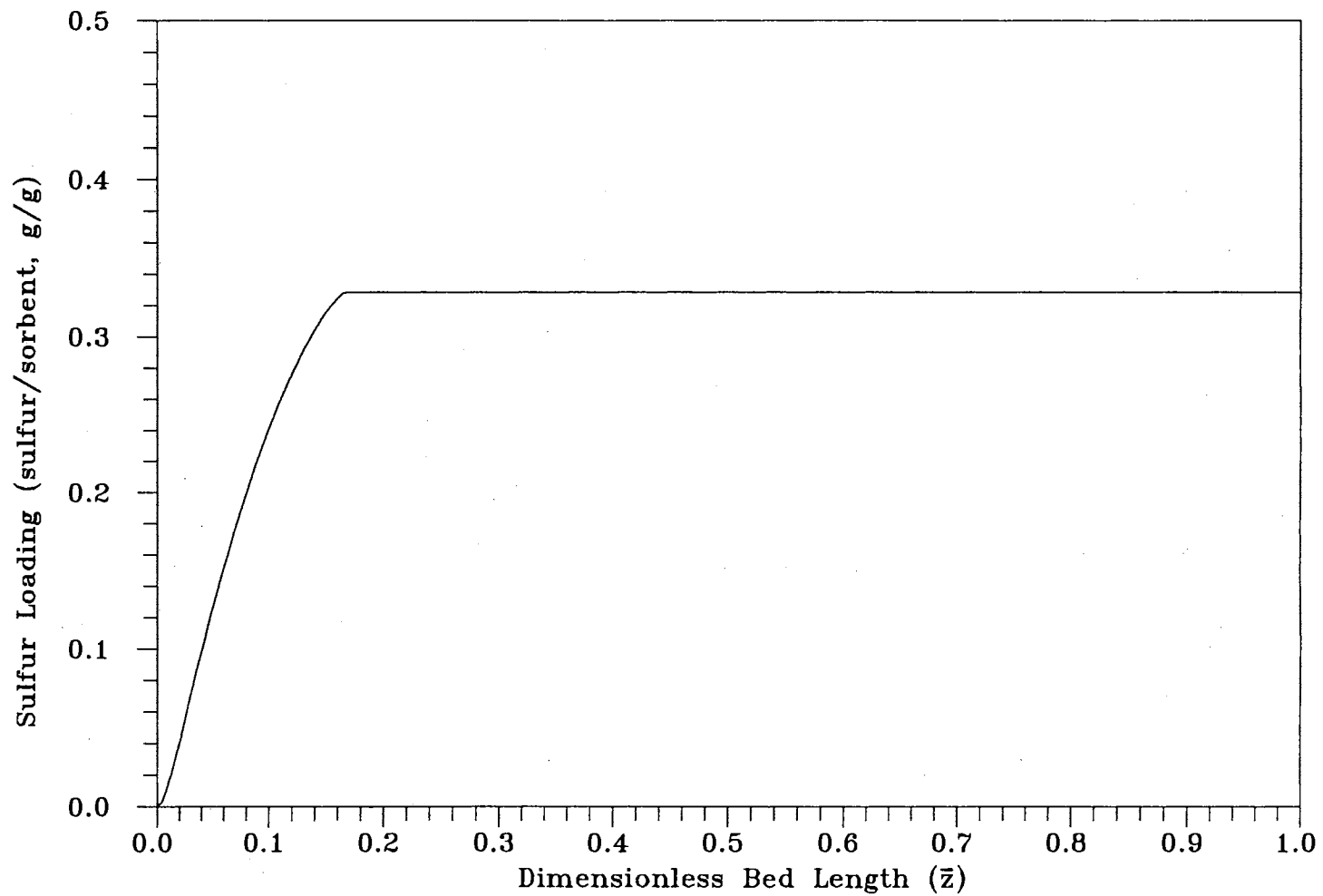


Figure 53. Initial Sulfur Loading Profile for Regeneration (pilot plant)

in Figure 54.

Figure 55 shows dimensionless gas temperature profiles in the regenerator at $t = 0.5, 1.0, 1.5$ and 2.0 hr. At these times, the gas and sorbent temperature profiles are compared in Figure 56. The traveling of the temperature profiles are presented in the above figures.

Figure 57 shows dimensionless gas temperature profiles at $t = 5, 10, 15, 20$ and 22 hr. The gas and sorbent temperature profiles are presented in Figure 58. After about 5 hours passed, the peak temperatures of the gas and sorbent approach to the almost same value.

Major differences (i.e., a sorbent utilization in the fixed-bed and temperature difference between gas and sorbent) of simulation results between the pilot plant scale system and the lab-scale system are attributed to following factors:

- 1) A higher heat transfer coefficient was used in the pilot plant scale system.
- 2) A higher gas-solid mass transfer coefficient was used in the simulation for the pilot plant scale system.
- 3) A higher superficial gas velocity was used in the pilot plant system.
- 4) The ratio of a reactor diameter versus reactor length in the pilot plant system is bigger than that in the lab- scale system.

In the two systems, values of operating temperatures, pressures, and concentrations (i.e., major parameters) were identical.

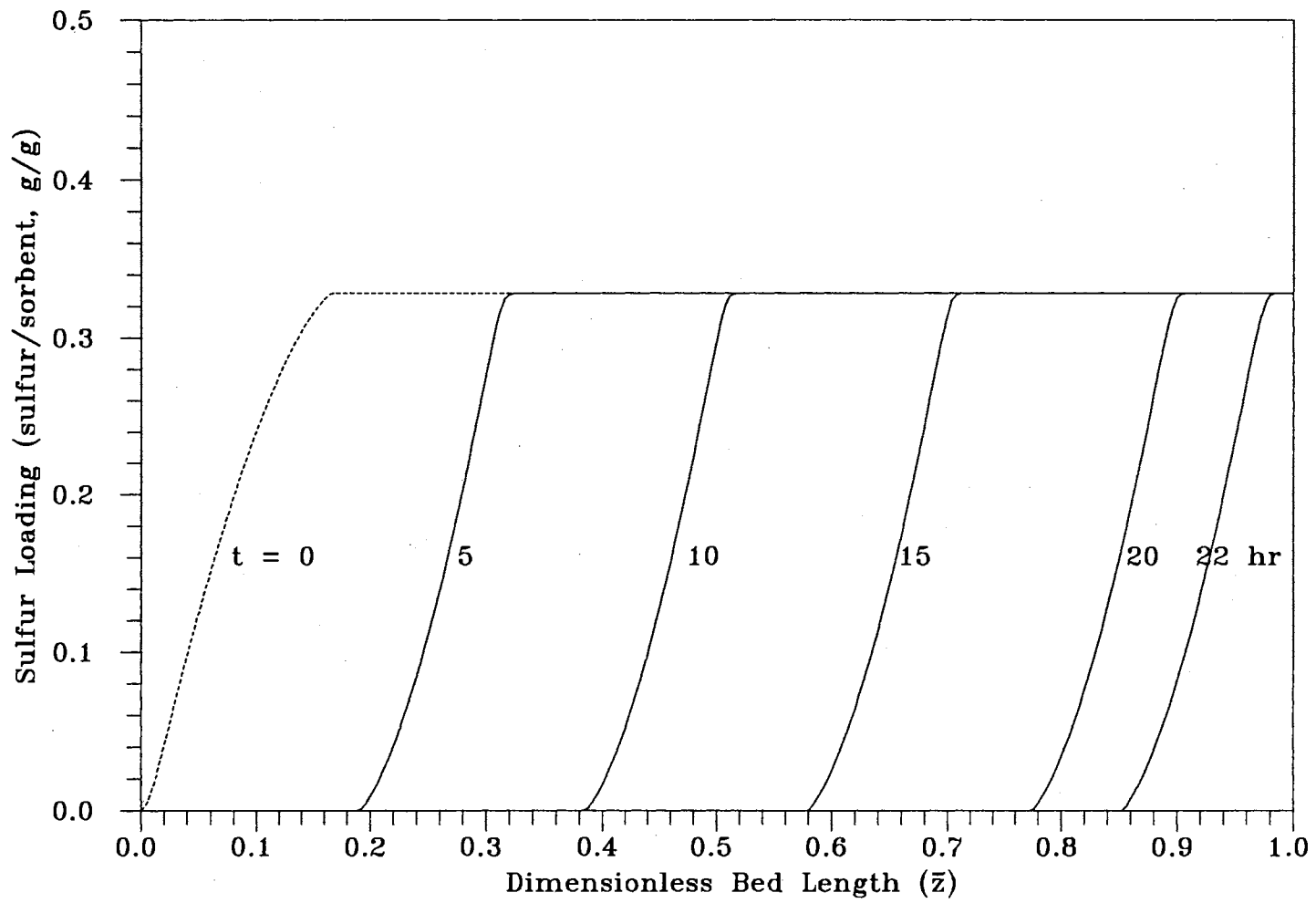


Figure 54. Sulfur Loading Profiles for Regeneration (pilot plant)

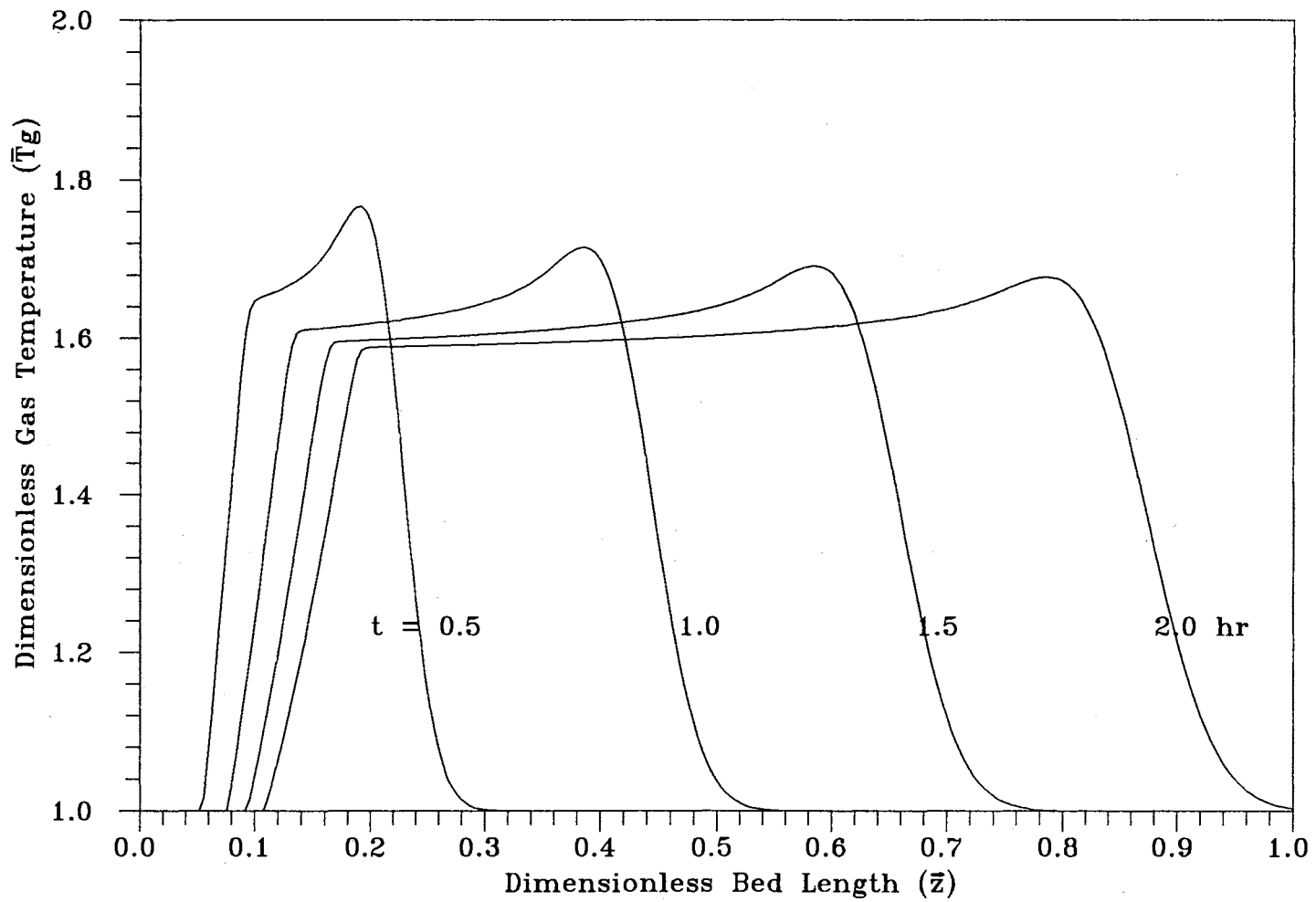


Figure 55. Dimensionless Gas Temperature Profiles for Regeneration (pilot plant)

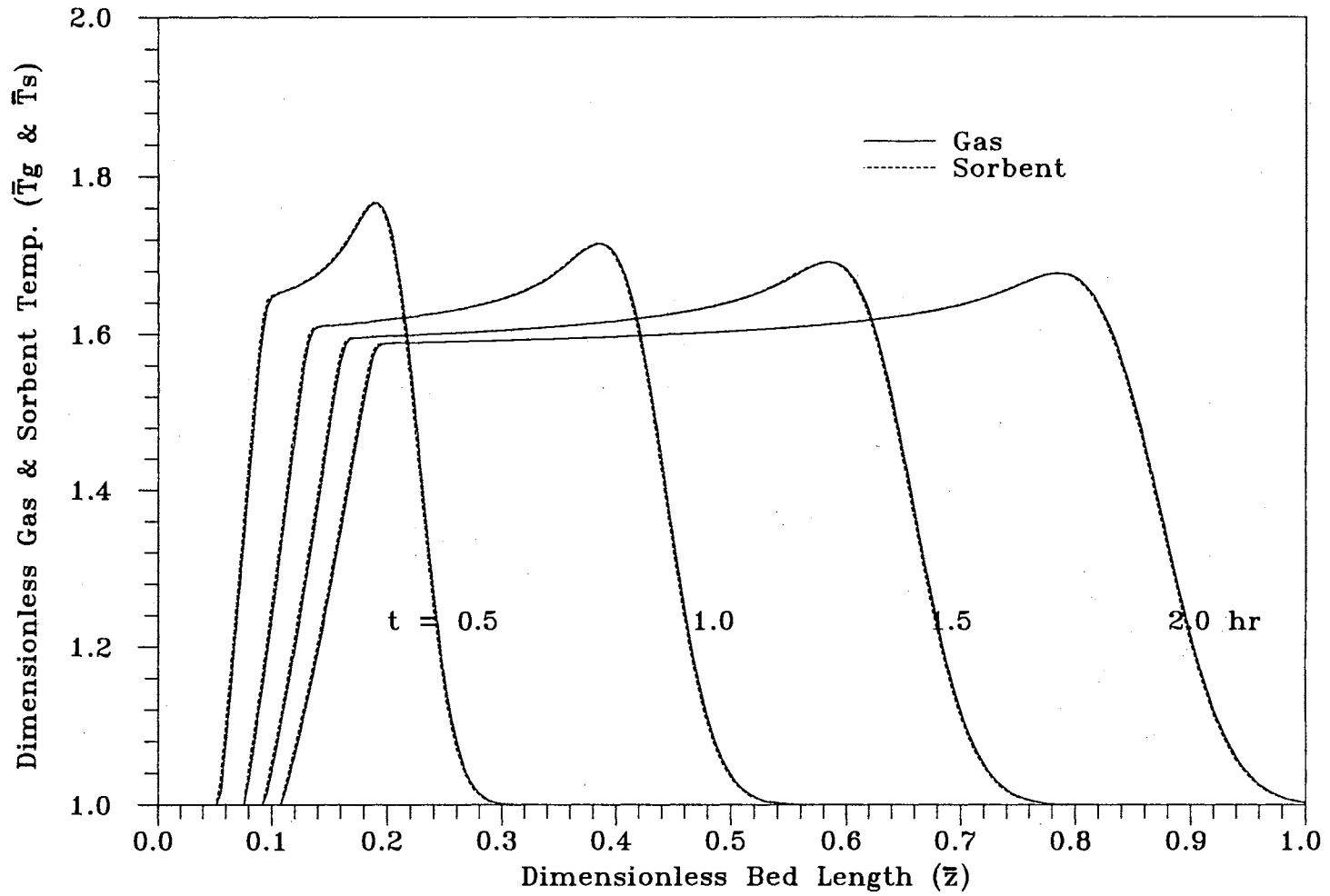


Figure 56. Dimensionless Gas & Sorbent Temperature Profiles for Regeneration (pilot plant)

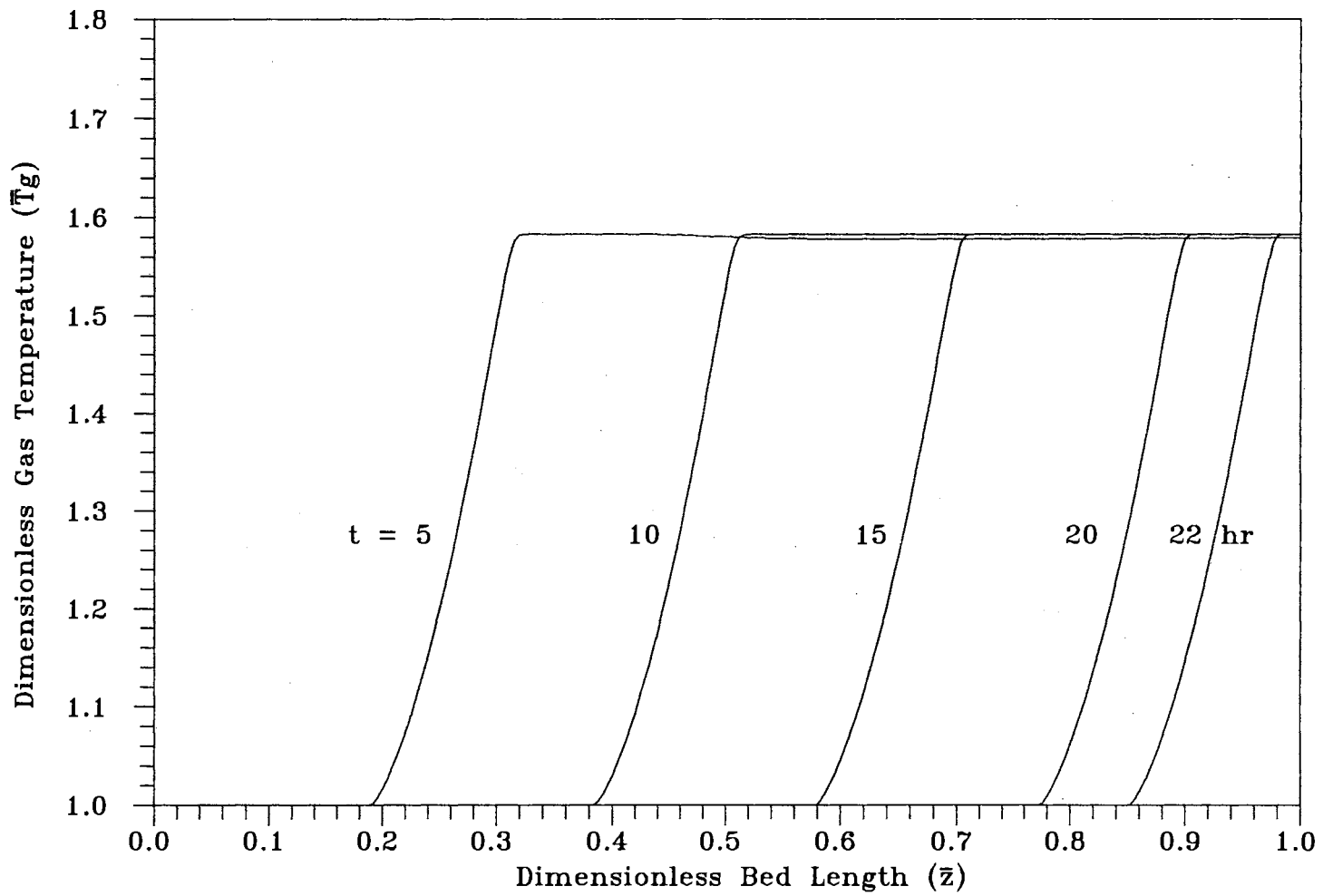


Figure 57. Dimensionless Gas Temperature Profiles for Regeneration (pilot plant; 5-22 hr)

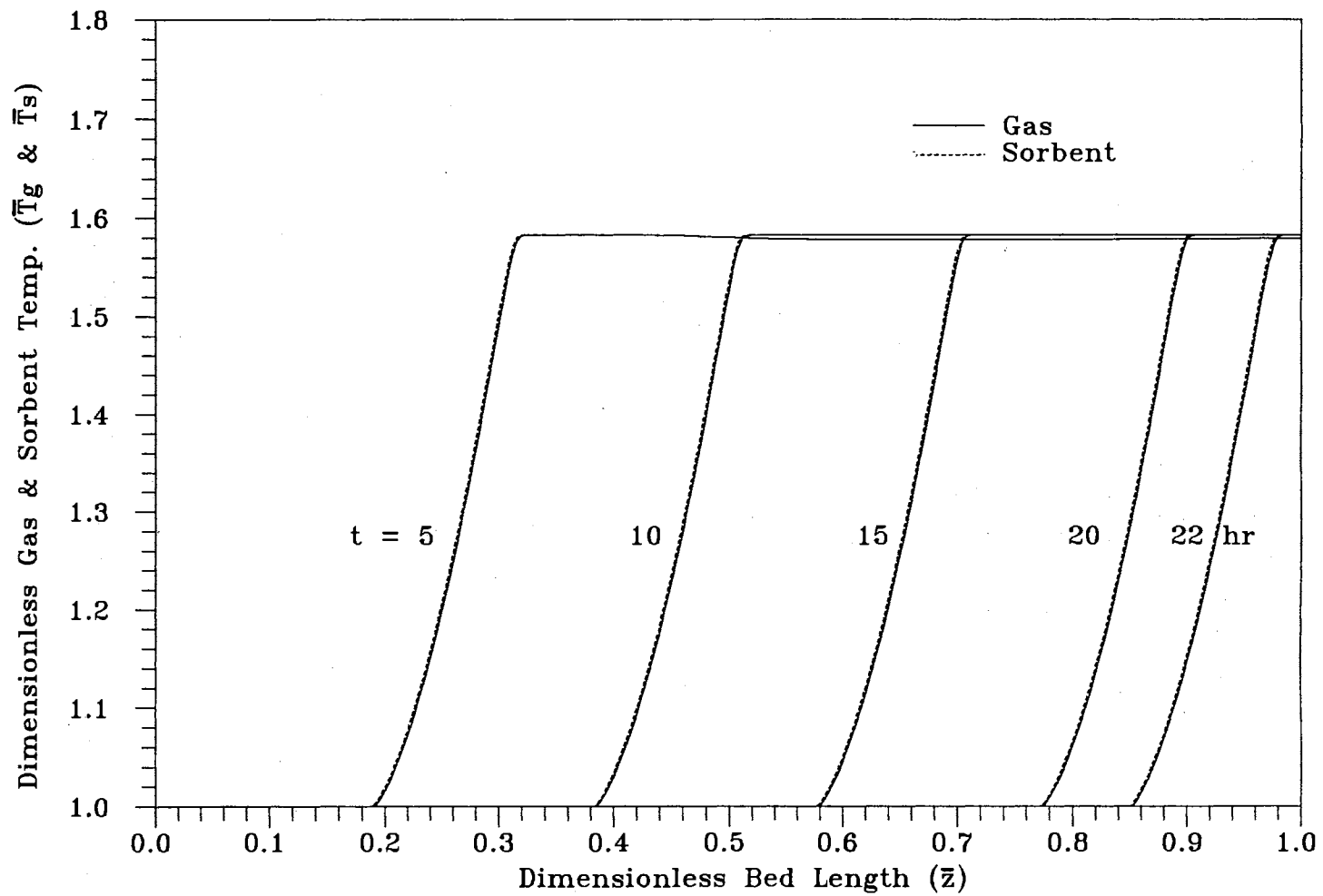


Figure 58. Dimensionless Gas & Sorbent Temperature Profiles for Regeneration (pilot plant; 5-22 hr)

CHAPTER VIII

CONCLUSIONS AND RECOMMENDATIONS

In this study, a mathematical model has been developed for the description of the unsteady state behavior of an adiabatic fixed-bed sulfidation-regeneration system. This system can be used for the clean-up of tail gas from the Claus bed and also for the increase of sulfur recovery efficiency in Claus plants. This model is the first to investigate a sulfidation-regeneration cycle by noncatalytic gas-solid reactions from a Claus tail gas clean-up viewpoint. Two dynamic simulation models (i.e., simulation programs for the sulfidation and regeneration) have been developed separately in order to test the performance of the developed mathematical model.

From the sulfidation simulation, the H_2S breakthrough curve was obtained as a function of the sulfidation time. Also, the following were predicted as a function of reactor axial position and time: H_2S gas concentration, sulfur loading of ZnO/Al_2O_3 sorbents, sorbent conversion, gas and sorbent temperatures. From the regeneration simulation, the O_2 breakthrough curve and the effluent SO_2 concentration profile have been predicted. Also, the following were predicted as a function of regenerator axial position and time: O_2 gas concentration, sulfur loading of ZnS/Al_2O_3 sorbents, gas and sorbent temperatures.

The following conclusions are drawn from simulation results of the sulfidation-regeneration fixed-bed reactors.

Conclusions

1) Inlet H_2S concentration showed a strong effect on the sulfidation breakthrough. Inlet gas temperature showed only a weak effect on the breakthrough curve. Superficial gas velocity had no effect on the slope of the breakthrough curve.

2) Higher superficial gas velocity results in faster regeneration, but the unreacted sulfur remains in a broader range in the regenerator. The higher the inlet O_2 concentration the less the amount of remaining sulfur in the regenerator. Inlet gas temperature had no effect on the sulfur loading profile for regeneration.

3) The higher the inlet O_2 concentration the higher the gas temperature rise in the regenerator. The same is true for the sorbent temperature rise. The inlet O_2 concentration and the regenerator operating temperature are very important factors for safe operation of the regenerator and for preventing sorbent sintering. A higher superficial gas velocity resulted in a lower gas temperature rise and increased the spread of gas temperature profile in the regenerator.

4) In the pilot plant scale system, the predicted temperature difference between the gas and the sorbent was smaller than that in the lab-scale system since a higher heat transfer coefficient was used in the pilot plant system.

5) The higher the gas-solid mass transfer coefficient used in the simulation for pilot plant system the better the utilization of sorbent than that in the lab-scale system. The effective diffusivities for both systems were almost identical.

Recommendations

1) The model predictions in this study were based on available literature correlations for physical parameters. Future work should use experimentally determined values for physical parameters (especially, for the effective diffusivity of the reactant gas in

the sorbent).

2) Comparison between the model predictions and experimental data should be made for model verification.

3) The extension of the model to handle multicycle operation of the sulfidation-regeneration system needs to be made with experimental sorbent conversion data.

4) The model itself can be refined by exclusion of some of the assumptions that were used in this study. These refinements would increase the amount of time required for a simulation.

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APPENDIXES

APPENDIX A

ESTIMATION OF MODEL PARAMETERS

Numerical values (shown in Table VII) of the following sulfidation model parameters are obtained or calculated from the industrial experimental conditions:

1. Bed diameter, D (cm): 167.6

2. Bed length, L (cm): 194.8

3. Bed voidage, ϵ_v (dimensionless): 0.4

4. Sorbent radius, R (cm): $(1/8 \text{ "})(0.5) = 0.1588 \text{ cm}$

5. Sorbent bulk density, ρ_s (g/cm³):

$$70.0 \text{ lbm/ft}^3 = 1.121 \text{ g/cm}^3$$

6. Sorbent charge, w (g):

$$\text{Bed volume} = \pi D^2 L / 4 = 4.298 \text{ E}+06 \text{ cm}^3$$

$$\text{Sorbent bulk density} = 1.121 \text{ g/cm}^3$$

$$\text{So, } w = (4.298 \text{ E}+06)(1.121) = 4.818 \text{ E}+06 \text{ g}$$

While, weight fraction of ZnO in the sorbent is 0.5. Hence, weight of ZnO in the bed is

$$(w)(0.5) = 2.409 \text{ E}+06 \text{ g}$$

7. Operating temperature, T (K): $800 \text{ }^\circ\text{F} = 700 \text{ K}$

Ranges of operating temperatures for the sulfidation reaction are from 650 to 1000 °F (i.e., from 633 to 811 K). 700 K is selected as an operating temperature in this example.

8. Operating pressure, P (atm): 1.05 atm

The sulfidation reactions are processed at this fixed operating pressure.

9. Superficial gas velocity (at operating T and P), U (cm/h):

$$56.85 \text{ ft/min} = 28.88 \text{ cm/s} = 1.04 \text{ E}+05 \text{ cm/h}$$

10. Volumetric gas flow rate (at operating T and P), v (cm³/h):

$$(\pi D^2 / 4) U = 6.368 \text{ E}+05 \text{ cm}^3/\text{s} = 2.294 \text{ E}+09 \text{ cm}^3/\text{h}$$

11. Initial molar concentration of H₂S, C_{Abo} (mol/cm³):

From the ideal gas assumption and the mole fraction of H₂S in the feed gas,

$$C_{\text{Abo}} = (P/R_g T)(Y_{\text{H}_2\text{S}})$$

where,

$$P = 1.05 \text{ atm}$$

$$R_g = 82.06 \text{ cm}^3 \cdot \text{atm/mol} \cdot \text{K}$$

$$T = 700 \text{ K}$$

$$Y_{\text{H}_2\text{S}} = 0.0188$$

So, $C_{\text{Abo}} = 3.437 \text{ E-07 mol H}_2\text{S/cm}^3$ feed gas

12. Initial molar concentration of ZnO, C_{Bo} (mol/cm³):

$$\begin{aligned} \text{particle density} &= (\text{bulk density})/(1 - \epsilon_v) \\ &= 1.121/(1-0.4) \\ &= 1.868 \text{ g/cm}^3 \end{aligned}$$

$$\text{molecular weight of ZnO} = 81.38 \text{ g/mol}$$

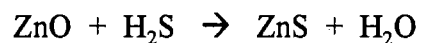
$$\text{ZnO fraction} = 0.5$$

Hence, $C_{\text{Bo}} = 1.868(0.5)/81.38 = 0.0115 \text{ mol/cm}^3$

Following parameters are estimated with literature data or correlations:

13. Heat of reaction (at operating T), ΔH (cal/mol):

For the sulfidation reaction,



the heat of reaction at 700 K is calculated as

$$\Delta H_{700\text{K}} = \Delta H_{298\text{K}} + \int_{298}^{700} (C_{p\text{ZnS}} + C_{p\text{H}_2\text{O}} - C_{p\text{ZnO}} - C_{p\text{H}_2\text{S}}) dT$$

In the above equation, the heat of reaction at 298 K (i.e., $\Delta H_{298\text{K}}$) is calculated from the standard heat of formation (at 25 °C) of each compound (Perry et al., 1984):

$$\Delta H_{f\text{ZnS}} = -45,300 \text{ cal/mol}$$

$$\Delta H_{f\text{H}_2\text{O}} = -57,797.9$$

$$\Delta H_{f\text{ZnO}} = -83,360$$

$$\Delta H_{f\text{H}_2\text{S}} = -4,770$$

Hence, $\Delta H_{298\text{K}} = -14,967.9 \text{ cal/mol}$

While, the heat capacity of each compound (Perry et al., 1984) is

$$C_{pZnS} = 12.81 + 0.00095T - 194600/T^2 \text{ cal/mol}\cdot\text{K}$$

$$C_{pH_2O} = 8.22 + 0.00015T + 0.00000134T^2$$

$$C_{pZnO} = 11.40 + 0.00145T - 182400/T^2$$

$$C_{pH_2S} = 33.51 + 1.547E-02T + 0.3012E-05T^2 - 3.292E-09T^3$$

The temperature for C_{pH_2S} is the Centigrade scale (Felder and Rousseau, 1986). Others are in Kelvin scale.

From these data,

$$\Delta H_{700K} = -14,617 \text{ cal/mol.}$$

14. Gas-solid mass transfer coefficient, k_m (cm/h):

Following data are required in order to use the correlation (6.1) in Chap VI:

a) Equivalent sorbent diameter, d_{pe} (cm):

The equivalent sorbent diameter used in the correlation (6.1) is the diameter of a sphere having the same external surface area as the sorbent in question. For a cylinder of length l and radius R , the equivalent sorbent diameter is

$$d_{pe} = (2Rl + 2R^2)^{1/2}$$

Thus, $d_{pe} = 0.5941 \text{ cm}$

b) Gas mass velocity, G (g/h·cm²):

From $G = (U)(\text{density of feed gas})$, $G = 83.28 \text{ g/h}\cdot\text{cm}^2$

c) Feed gas viscosity, μ (g/cm·s):

The viscosities of pure gases at operating T and P are calculated from the following equation (Reid et al., 1987):

$$\mu = [(2.6693 \text{ E-}05)(M\cdot T)^{1/2}]/[\sigma^2\cdot\Omega]$$

For CO_2 ,

$$\epsilon^*/k^* = 195.2 \text{ K}$$

$$\sigma = 3.941 \text{ Angstroms}$$

$$M = 44.01$$

$$\Omega = 0.9937$$

thus, $\mu_{\text{CO}_2} = 3.036 \text{ E-04 g/cm}\cdot\text{s}$

For H_2S ,

$$\varepsilon^*/k^* = 301.1 \text{ K}$$

$$\sigma = 3.623 \text{ Angstroms}$$

$$M = 34.08$$

$$\Omega = 1.119$$

thus, $\mu_{\text{H}_2\text{S}} = 2.807 \text{ E-04 g/cm}\cdot\text{s}$

While, the viscosity of gas mixture can be calculated by the method of Wilke (Reid et al, 1987):

For binary system,

$$\mu = \frac{Y_1\mu_1}{Y_1 + Y_2\Phi_{12}} + \frac{Y_2\mu_2}{Y_2 + Y_1\Phi_{21}}$$

where,

$$\Phi_{12} = \frac{\left(1 + (\mu_1 / \mu_2)^{1/2} (M_2 / M_1)^{1/4}\right)^2}{\left(8(1 + (M_1 / M_2))\right)^{1/2}}$$

$$\Phi_{21} = \Phi_{12} \frac{\mu_2 M_1}{\mu_1 M_2}$$

In the above equations,

Y_1 = mole fraction of H_2S

Y_2 = mole fraction of CO_2

μ_1 = viscosity of H_2S

μ_2 = viscosity of CO₂

M_1 = molecular weight of H₂S

M_2 = molecular of CO₂

From these data, the feed gas viscosity is

$$\mu = 3.032 \text{ E-04 g/cm}\cdot\text{s}$$

d) Reynolds number, Re_p :

$$Re_p = d_{pe} \cdot G / \mu = 45.33$$

e) Schmidt number, Sc :

$$Sc = \mu / (\text{feed gas density}) \cdot D_{AB} = 0.692$$

f) Sherwood number, Sh :

$$Sh = 2 + 1.1(Sc)^{1/3}(Re_p)^{0.6} = 11.6 = k_m \cdot d_{pe} / D_{AB}$$

From the above data,

$$k_m = 38,426 \text{ cm/h}$$

15. Gas-solid heat transfer coefficient, h (cal/cm²·h·K):

From the correlation (6.5) in Chap VI and other data,

$$Nu = 0.36(Re_p)^{0.94} = 12.98$$

$$Nu = h \cdot d_{pe} / k$$

$$k_{CO_2} = 0.0481 \text{ W/m}\cdot\text{K (Perry et al., 1984)}$$

$$k_{H_2S} = \text{from the chart in Engineering Data Book (GPSA, Tulsa, OK 1987)}$$

k = thermal conductivity of the feed gas

The value of h is

$$2.508 \text{ E-03 cal/s}\cdot\text{cm}^2\cdot\text{K} = 9.036 \text{ cal/h}\cdot\text{cm}^2\cdot\text{K}$$

16. Effective diffusivity within the sorbent, D_e (cm²/h):

In Eq. (6.11),

$$r^* = 1.156 \text{ E-06 cm}$$

$$T = 700 \text{ K}$$

$$M = 34.08 \text{ (for H}_2\text{S)}$$

Therefore, $D_K = 5.082 \text{ E-02 cm}^2/\text{s}$

In Eq. (6.12),

$$T = 700 \text{ K}$$

$$P = 1.05 \text{ atm} = 1.064 \text{ bar}$$

$$\sigma_{AB} = (\sigma_A + \sigma_B)/2$$

$$\sigma_A = 3.623 \text{ Angstroms (for H}_2\text{S)}$$

$$\sigma_B = 3.941 \text{ Angstroms (for CO}_2\text{)}$$

$$\Omega_D = 0.9599 \text{ (from the relation of Neufield et al., 1972 (Reid et al., 1987))}$$

Therefore, $D_{AB} = 0.5471 \text{ cm}^2/\text{s}$

From Eq. (6.10) with D_K and D_{AB} ,

$$D_c = 0.04649 \text{ cm}^2/\text{s}$$

Finally, from Eq. (6.9),

$$D_c = 0.01666 \text{ cm}^2/\text{s} = 59.96 \text{ cm}^2/\text{h}$$

17. Average heat capacity of the feed gas, C_{pg} (cal/g-K):

From the mole fractions of H_2S and CO_2 and the following correlations (T in $^\circ\text{C}$; C_p in $\text{J/mol}\cdot^\circ\text{C}$),

$$C_{p\text{CO}_2} = 36.11 + (4.233 \text{ E-02})T - (2.887 \text{ E-05})T^2 + (7.464 \text{ E-09})T^3$$

$$C_{p\text{H}_2\text{S}} = 33.51 + (1.547 \text{ E-02})T + (0.3012 \text{ E-05})T^2 - (3.292 \text{ E-09})T^3$$

Thus, the value of C_{pg} is $0.2691 \text{ cal/g}\cdot\text{K}$

18. Average heat capacity of the solid sorbent, C_{ps} (cal/g-K):

From the weight fractions of Al_2O_3 and ZnO and the following correlations (Perry et al., 1984; T in K),

$$C_{p\text{Al}_2\text{O}_3} = 22.08 + 0.008971T - 522500/T^2$$

$$C_{p\text{ZnO}} = 11.4 + 0.00145T - 182400/T^2$$

the value of C_{ps} is $0.2078 \text{ cal/g}\cdot\text{K}$

APPENDIX B

PROGRAM FOR SULFIDATION MODEL

C ***** ABSTRACT *****

C

C This program can be used to simulate a noncatalytic

C gas-solid sulfidation reaction ($ZnO+H_2S \rightarrow ZnS+H_2O$)

C in an adiabatic fixed-bed reactor. Following

C simulation results can be used to design and/or develop

C a tail-gas clean-up process for the efficient removal

C of H_2S from Claus-bed:

C 1) H_2S breakthrough curve

C 2) H_2S gas concentration profiles

C 3) Sorbent conversion profiles

C 4) Sulfur loading profiles

C 5) Gas temperature profiles

C 6) Sorbent temperature profiles

C A shrinking core model is selected to describe the

C kinetics of a single sorbent in the reactor. One

C dimensional heterogeneous model is used for the

C description of the adiabatic fixed-bed reactor.

C The dimensionless governing equations are

C integrated using the fourth order Adams-Moulton

C predictor-corrector method.

C

C *****

C -----

C NOMENCLATURE FOR THE SULFIDATION PROGRAM

C -----

C

C D : FIXED-BED DIAMETER (cm)

C L : FIXED-BED LENGTH (cm)

C BV : BED VOIDAGE (DIMENSIONLESS)

C R : SORBENT RADIUS (cm)

C SBDEN : SORBENT BULK DENSITY (g/cm³)

C BVOL : BED VOLUME (cm³)

C W : SORBENT CHARGE FOR ZNO/AL₂O₃ (g)

C WSOB : SORBENT CHARGE FOR ZNO (g)

C TEM : OPERATING TEMPERATURE (K)

C P : OPERATING PRESSURE (atm)

C U : SUPERFICIAL GAS VELOCITY AT TEM & P (cm/h)

C V : VOLUMETRIC GAS FLOW RATE (cm³/h)

C Y1 : MOLE FRACTION OF H_2S (dimensionless)

C RG : GAS CONSTANT (cm³ atm/K mol)

C CAB0 : INITIAL CONC. OF H_2S (mol/cm³)

C CBO : INITIAL CONC. OF ZNO (mol/cm³)

C DELH : HEAT OF REACTION AT TEM (cal/mol)

C CYLEN : LENGTH OF A CYLINDRICAL SORBENT (cm)

C DPE : EQUIVALENT SORBENT DIAMETER (cm)

C G : GAS MASS FLOW RATE (g/h cm²)

C TV1,TV2 : DIMENSIONLESS TEMPERATURES FOR H_2S & CO_2

C (=TEM*Boltzmann's const./characteristic

C energy)

C OM1,OM2 : VISCOSITY COLLISION INTEGRALS FOR H_2S & CO_2

C CALCULATED BY NEUFELD ET AL.' EQUATION

C (dimensionless)

```

C VIS1,VIS2 : VISCOSITIES FOR H2S & CO2 CALCULATED BY
C CHAPMAN-ENSKOG EQUATION (g/cm s)
C PI12,PI21 : FACTORS USED IN WILKE'S EQUATION
C (dimensionless)
C VISM : VISCOSITY OF THE MIXTURE CALCULATED BY
C WILKE'S EQUATION (g/cm s)
C SIG12 : CHARACTERISTIC LENGTH (Angstroms)
C TV3 : DIMENSIONLESS TEMPERATURE USED IN OMD
C OMD : DIFFUSION COLLISION INTEGRAL CALCULATED BY
C NEUFELD ET AL.' EQUATION (dimensionless)
C D12 : DIFFUSION COEFFICIENT FOR BINARY GAS SYSTEM
C (cm2/s)
C REP : PARTICLE REYNOLDS NUMBER (dimensionless)
C SC : SCHMIDT NUMBER (dimensionless)
C SH : SHERWOOD NUMBER (dimensionless)
C NU : NUSSELT NUMBER (dimensionless)
C KM : GAS-SOLID MASS TRANSFER COEFFICIENT
C CALCULATED BY WAKAO & FUNAZKRI'S EQUATION
C (cm/h)
C KS : RATE CONSTANT
C H : GAS-SOLID HEAT TRANSFER COEFFICIENT
C CALCULATED BY GLIDDON & CRANFIELD'S
C EQUATION (cal/cm2 h K)
C DK : KNUDSEN DIFFUSIVITY (cm2/s)
C DC : COMBINED DIFFUSIVITY (cm2/s)
C DE1 : EFFECTIVE DIFFUSIVITY OF H2S WITHIN THE
C SORBENT (cm2/h)
C CPG1,CPG2 : HEAT CAPACITIES FOR H2S & CO2 (cal/g K)
C CPGM : AVERAGE HEAT CAPACITY OF GAS (cal/g K)
C CPS1,CPS2 : HEAT CAPACITIES FOR ZNO & AL2O3 (cal/g K)
C CPSM : AVERAGE HEAT CAPACITY OF SORBENT (cal/g K)
C
C -----

```

```

C ***** MAIN SULFIDATION PROGRAM *****

```

```

REAL L,M1,M2,M12,KM,NU,KS

```

```

COMMON /COM1/ INUM
COMMON /COM2/ FC2
COMMON /COM3/ FC1
COMMON /COM4/ FC3, FC4
COMMON /COM6/ FCRBV
COMMON /COM7/ FCBTA1, FCBTA3, FCBTA2, DE1, R
COMMON /COM8/ TSLOAD
COMMON /COM9/ CABPPM
COMMON /COM10/ BKPPM

```

```

C ----- LIST AND COMPUTATION OF INPUT DATA (FOR MODEL
C PARAMETERS AND SECONDARY PARAMETERS)

```

```

D = 4.09
L = 19.48
BV = 0.4

```

R = 0.1588
SBDEN = 1.121

BVOL = 3.1416*D**2*L/4.
W = BVOL*SBDEN
WSOB = 0.5*W

TEM = 700.
P = 1.05

USTPFM = 0.3*25.41195
USTPCH = USTPFM*0.00508*100.*3600.
U = USTPCH*(TEM/298.)*(1./P)
V = U*3.1416*D**2/4.

Y1 = 0.0188
RG = 82.06
CABPPM = Y1*(1.E6)
CABO = Y1*P/RG/TEM
CBO = 0.5*SBDEN/(1.-BV)/81.38

B = 1.0

DELH = -14967.9 + 9.63*(TEM-298.) - (1.75E-4)*(TEM**2
* -298.**2)+(1.22E4)*(1./TEM - 1./298.) +
* ((1.34E-6)/3.)*(TEM**3-298.**3) - 0.239006*
* (33.51*(TEM-273.-25.)+(1.547E-2/2.)*((TEM-273.)
* **2-25.**2)+(0.3012E-5/3.)*((TEM-273.)**3
* -25.**3)-(3.292E-9/4.)*((TEM-273.)**4-25.**4))

CYLEN = 0.9525
DPE = (2.*R*CYLEN + 2.*R**2)**0.5
M1 = 34.08
M2 = 44.01
G = (P/RG/TEM)*(M1*Y1 + M2*(1. - Y1))*U

TV1 = TEM/301.1
AA = 1.16145
BB = 0.14874
CC = 0.52487
DD = 0.7732
EE = 2.16178
FF = 2.43787
OM1 = AA*TV1**(-BB)+CC*(EXP(-DD*TV1))+EE*
* (EXP(-FF*TV1))
VIS1 = (2.6693E-5)*((M1*TEM)**0.5)/3.623**2/OM1

TV2 = TEM/195.2
OM2 = AA*TV2**(-BB)+CC*(EXP(-DD*TV2))+EE*
* (EXP(-FF*TV2))
VIS2 = (2.6693E-5)*((M2*TEM)**0.5)/(3.941**2)/OM2

PI12 = (1.+((VIS1/VIS2)**0.5)*(M2/M1)**0.25)**2 /
* (8.*(1.+(M1/M2)))**0.5
PI21 = PI12*VIS2*M1/VIS1/M2

```

VISM = Y1*VIS1/(Y1+(1.-Y1)*PI12) +
*      (1.-Y1)*VIS2/((1.-Y1)+Y1*PI21)

M12 = 2./(1./M1 + 1./M2)
SIG12 = (3.623+3.941)/2.
TV3 = TEM/(301.1*195.2)**0.5
OMD = 1.06036/TV3**0.1561 + 0.193/EXP(0.47635*TV3)
*      + 1.03587/EXP(1.52996*TV3)
*      + 1.76474/EXP(3.89411*TV3)
D12 = 0.00266*TEM**1.5/(P*1.0133)/(M12**0.5)/
*      (SIG12**2)/OMD

REP = DPE*G/3600./VISM
SC = VISM/D12/(G/U)
SH = 2. + 1.1*(SC**(1./3.))*(REP**0.6)
NU = 0.36*REP**0.94

KM = 3600.*SH*D12/DPE

H = 3600.*NU*(1.1488E-4)/DPE

DK = (9.7E3)*(1.156E-6)*(TEM/M1)**0.5
DC = DK*D12/(DK + D12)
DE1 = 3600.*DC*(1.-((SBDEN/(1.-BV))/4.653))**2

CPG1 = (33.51 + (1.547E-2)*(TEM-273.) +
*      (0.3012E-5)*(TEM-273.)**2 - (3.292E-9)*
*      (TEM-273.)**3)*0.239006/M1
CPG2 = (36.11 + (4.233E-2)*(TEM-273.) -
*      (2.887E-5)*(TEM-273.)**2 + (7.464E-9)*
*      (TEM-273.)**3)*0.239006/M2
CPGM = Y1 * CPG1 + (1.-Y1)*CPG2

CPS1 = (22.08 + 0.008971*TEM - 522500./(TEM**2))/
*      101.963
CPS2 = (11.4 + 0.00145*TEM - 182400./(TEM**2))/
*      81.38
CPSM = 0.5*CPS1 + 0.5*CPS2

KS = 4.E8
ASV = 2.*(1.-BV)/R

```

C ----- COMPUTATION OF FACTORS IN FUNCTION BETA

```

FCBTA1 = 2.*(1.-BV)/(U/L)
FCBTA2 = R/KM
FCBTA3 = R/(KS*CB0)

```

C ----- COMPUTATION OF A FACTOR IN FUNCTION RBV

```

FCRBV = (U/L)*B*CAB0/(1.-BV)

```

C ----- COMPUTATION OF FACTORS IN DIMENSIONLESS
C GOVERNING EQUATIONS

```

FC1 = CABO*B*U/(CBO*L*(1.-BV))
FC2 = H*ASV*L/(G*CPGM)
FC3 = -DELH/(SBDEN/(1.-BV))/CPSM/TEM
FC4 = H*ASV/(1.-BV)/(SBDEN/(1.-BV))/CPSM

```

```

C ----- TIME OF BREAKTHROUGH FOR COMPLETE SULFIDATION
C           OF A FRESH BED

```

```

TOSRXT = BVOL*(1.-BV)*CBO
BKTCMS = TOSRXT/(V*CABO)/B

```

```

WRITE(6,22) BKTCMS
22  FORMAT(//2X, ' TIME FOR COMPLETE SULFIDATION'
*      / 2X, ' OF A FRESH BED = ',E10.2, 'hr')

```

```

C ----- THEORETICAL SULFUR LOADING FOR A FRESH SORBENT

```

```

C      TSLOAD = CBO*32./(0.5*SBDEN/(1.-BV))/B
C      WRITE(6,24) TSLOAD
C 24  FORMAT(//2X, ' THEORETICAL SULFUR LOADING = ',F8.4,
C      *      ' WT S PER WT FRESH SORBENT')

```

```

C ----- THEORETICAL SULFUR LOADING FOR A SULFIDED
C           SORBENT

```

```

TSLOAD = CBO*32./(0.5*SBDEN/(1.-BV))/B/(97.44/81.38)
WRITE(6,26) TSLOAD
26  FORMAT(//2X, ' THEORETICAL SULFUR LOADING = ',F8.4,
*      ' WT S PER WT SULFIDED SORBENT')

```

```

C ----- STEP SIZES OF TIME AND Z FOR THE INTEGRATION
C           OF DIMENSIONLESS GOVERNING EQUATIONS

```

```

DLT = 0.002
INUM = 250
DLZ = 1./INUM
INUM = INUM + 1

```

```

C
C      TBGIN = 0.002
C      TINT = 0.002
C      TEND = 0.002

```

```

C -----
C
C      BBGIN = 0.1
C      BINT = 0.1
C      BEND = 1.0

```

```

C
C -----
C
C      WRITE(6,28)
28  FORMAT(// ' ENTER H2S BREAKTHROUGH (PPM): ' )

```

```

      READ(5,*) BKPPM
C
C ----- ENTER THE SIMULATION TIME FOR SULFIDATION
      CALL SULTIME (TBGIN, TINT, TEND)
C ----- CALL ADAMS-MOULTON 4TH ORDER METHOD FOR THE
C           INTEGRATION OF DIMENSIONLESS GOVERNING
C           EQUATIONS
      CALL AMPC (DLZ,DLT,TBGIN,TINT,TEND,BBGIN,BINT,BEND)

      STOP
      END

C ***** END OF MAIN PROGRAM *****
C ***** SUBROUTINE SULTIME *****

      SUBROUTINE SULTIME (TBGIN, TINT, TEND)
      COMMON /COM1/ INUM

39  WRITE (6,35)
35  FORMAT (/ ' ENTER BEGINNING, INTERVAL AND ENDING '
*/' TIME FOR SULFIDATION SIMULATION (hr):')
      READ (5,*) TBGIN,TINT,TEND

      IF ((TBGIN.GT.TEND).OR.(TINT.GT.TEND)) THEN
          WRITE (6,36)
36  FORMAT ('OOOOOPS ! PLEASE ENTER AGAIN !')
          GO TO 39
      END IF

      IF(ABS(TBGIN).LE.1.E-2) TBGIN = TINT

      RETURN
      END

C ***** SUBROUTINE AMPC *****

C ----- USE ADAMS-MOULTON 4TH ORDER METHOD FOR THE
C           INTEGRATION OF DIMENSIONLESS GOVERNING
C           EQUATIONS

      SUBROUTINE AMPC(DLZ,DLT,TBGIN,TINT,TEND,BBGIN,BINT,
*           BEND)

      LOGICAL BKTIME

      DIMENSION Z(251),TG(251),TS(251),CAB(251),X(251),
*           BKSX(251)

```



```

DIMENSION TS1(251),TG1(251),X1(251),CAB1(251)
DIMENSION TS2(251),TG2(251),X2(251),CAB2(251)
DIMENSION TS3(251),TG3(251),X3(251),CAB3(251)
DIMENSION SULCAB(12550),SULX(12550),SULTG(12550),
*      SULTS(12550),SULOAD(12550),PPMEXT(12550)
DIMENSION IBPNT(10),TGIMSI(10,50),TSIMSI(10,50),
*      BTG(500),BTS(500)

```

```

COMMON /COM1/ INUM
COMMON /COM2/ FC2
COMMON /COM3/ FC1
COMMON /COM4/ FC3,FC4
COMMON /COM6/ FCRBV
COMMON /COM7/ FCBTA1,FCBTA3,FCBTA2,DE1,R
COMMON /COM8/ TSLoad
COMMON /COM9/ CABPPM
COMMON /COM10/ BKPPM

```

```

C -----
C -----

```

```

      BKTIME = .FALSE.

```

```

C -----

```

```

      NBLIN = INT((BEND-BBGIN)/BINT*1.001) + 1
      IBPNT(1) = INT((INUM-1)*BBGIN*1.0001) + 1
      DO 500 IBED = 1,NBLIN-1
500      IBPNT(IBED+1) = INT((INUM-1)*(BBGIN+BINT*IBED)
*      *1.0001) + 1

      NT = 1
      NTIME = 50
      BTBGIN = TEND/NTIME
      BDEPSI = 0.5*BTBGIN

```

```

C -----

```

```

      EPSI = 1.E-50
      EPS = 0.5*DLT
      T = 0.
      PPMEXT(1) = 0.

```

```

      Z(1) = 0.

```

```

      DO 41 I = 1, INUM-1

```

```

          Z(I+1) = Z(I) + DLZ

```

```

41      CONTINUE

```

```

C ----- INITIAL CONDITIONS FOR THE INTEGRATION OF
C      DIMENSIONLESS GOVERNING EQUATIONS

```

```

      CAB(1) = 1.

```

```

TG(1) = 1.

DO 42 I = 1, INUM

    X(I) = 0.
    TS(I) = 1.

42 CONTINUE

C -----
    WRITE (6,300)
300 FORMAT(// ' PLEASE WAIT FOR SIMULATION RESULTS !' )

C -----
C ----- COMPUTE AT THE FOLLOWING GRID POINT:
C          (i,j) = (2,1)

    CABSE = CAB(1) + DLZ*FN1(X(1),CAB(1))
    IF(CABSE.LT.EPSI) CABSE = EPSI
    IF(CABSE.GT.1.0) CABSE = 1.0

    TGSE = TG(1) + DLZ*FN2(TS(1),TG(1))

    CAB(2) = CAB(1) + 0.5*DLZ*(FN1(X(1),CAB(1))
*          +FN1(X(2),CABSE))
    TG(2) = TG(1) + 0.5*DLZ*(FN2(TS(1),TG(1))
*          + FN2(TS(2),TGSE))

C ----- COMPUTE AT: (i,j) = (3,1) & (4,1)

    DO 51 I = 3,4

        CABPD = CAB(I-2)+2.0*DLZ*FN1(X(I-1),CAB(I-1))
        TGPD = TG(I-2)+2.0*DLZ*FN2(TS(I-1),TG(I-1))
        IF(ABS(CABPD).LE.EPSI) CABPD = EPSI
        CAB(I) = CAB(I-1)+0.5*DLZ*(FN1(X(I-1),CAB(I-1))
*          + FN1(X(I),CABPD))
        TG(I) = TG(I-1)+0.5*DLZ*(FN2(TS(I-1),TG(I-1))
*          + FN2(TS(I),TGPD))
        IF(ABS(CAB(I)).LT.EPSI) CAB(I) = EPSI

51 CONTINUE

C ----- COMPUTE AT: (i,j) = FROM (5,1) TO (INUM,1)

    DO 52 I = 5, INUM

        CABPD = CAB(I-1)+(DLZ/24.)*(55.*FN1(X(I-1),CAB(I-1))
*          -59.*FN1(X(I-2),CAB(I-2))+37.*FN1(X(I-3),
*          CAB(I-3))-9.*FN1(X(I-4),CAB(I-4)))
        TGPD = TG(I-1)+(DLZ/24.)*(55.*FN2(TS(I-1),TG(I-1))
*          -59.*FN2(TS(I-2),TG(I-2))+37.*FN2(TS(I-3),
*          TG(I-3))-9.*FN2(TS(I-4),TG(I-4)))
        IF(ABS(CABPD).LE.EPSI) CABPD = EPSI

```

```

      CAB(I) = CAB(I-1)+(DLZ/24.)*(9.*FN1(X(I),CABPD)
*       +19.*FN1(X(I-1),CAB(I-1))-5.*FN1(X(I-2),
*       CAB(I-2))+FN1(X(I-3),CAB(I-3)))
      TG(I) = TG(I-1)+(DLZ/24.)*(9.*FN2(TS(I),TGPD)
*       +19.*FN2(TS(I-1),TG(I-1))-5.*FN2(TS(I-2),
*       TG(I-2))+FN2(TS(I-3),TG(I-3)))
      IF(ABS(CAB(I)).LT.EPSI) CAB(I) = EPSI

```

52 CONTINUE

```

C -----
C----- GOING TO THE NEXT TIME STEP
C ----- COMPUTE AT: (i,j) = (1,2)

```

```

      XSE = X(1) + FN3(X(1),CAB(1))*DLT
      IF(XSE.LT.EPSI) XSE = EPSI
      IF(XSE.GT.1.) XSE = 1.0
      TSSE = TS(1) + FN4(TS(1),TG(1),X(1),CAB(1))*DLT

```

```

      XCT = X(1)+0.5*DLT*(FN3(X(1),CAB(1))+FN3(XSE,CAB(1)))
      TSCT = TS(1) + 0.5*DLT*(FN4(TS(1),TG(1),X(1),CAB(1))
*       +FN4(TSSE,TG(1),XSE,CAB(1)))
      IF(XCT.LT.EPSI) XCT = EPSI
      IF(XCT.GT.1.) XCT = 1.0

```

```

      X1(1) = X(1)
      TS1(1) = TS(1)
      X(1) = XCT
C      IF(X(1).GT.XRVNW(1)) X(1) = 1.
      TS(1) = TSCT

```

C ----- COMPUTE AT: (i,j) = (2,2)

```

      TSSE = TS(2) + DLT*FN4(TS(2),TG(2),X(2),CAB(2))
      XSE = X(2) + DLT*FN3(X(2),CAB(2))
      CABSE = CAB(1) + DLZ*FN1(X(1),CAB(1))
      IF(ABS(CABSE).LT.EPSI) CABSE = EPSI
      IF(ABS(XSE).LT.EPSI) XSE = EPSI
      TGSE = TG(1) + DLZ*FN2(TS(1),TG(1))

```

```

      TSCT = TS(2) + 0.5*DLT*(FN4(TS(2),TG(2),X(2),CAB(2))
*       +FN4(TSSE,TGSE,XSE,CABSE))
      XCT = X(2)+0.5*DLT*(FN3(X(2),CAB(2))+FN3(XSE,CABSE))
      CABCT = CAB(1)+0.5*DLZ*(FN1(X(1),CAB(1))
*       +FN1(XSE,CABSE))

```

```

      IF(ABS(CABCT).LT.EPSI) CABCT = EPSI
      IF(ABS(XCT).LT.EPSI) XCT = EPSI
      TGCT = TG(1)+0.5*DLZ*(FN2(TS(1),TG(1))+
*       FN2(TSSE,TGSE))

```

```

C
      X1(2) = X(2)
      TS1(2) = TS(2)
      CAB1(2) = CAB(2)

```

```

      TG1(2) = TG(2)
      X(2) = XCT
C      IF(X(2).GT.XRVNW(2)) X(2)=1.
      TS(2) = TSCT
      CAB(2) = CABCT
      TG(2) = TGCT

C ----- COMPUTE AT: (i,j) = (3,2) & (4,2)

      DO 53 I = 3,4

          XSE = X(I) + DLT*FN3(X(I),CAB(I))
          TSSE = TS(I) + DLT*FN4(TS(I),TG(I),X(I),CAB(I))
          IF(ABS(XSE).LT.EPSI) XSE = EPSI

          TGPD = TG(I-2)+2.0*DLZ*FN2(TS(I-1),TG(I-1))
          CABPD = CAB(I-2)+2.0*DLZ*FN1(X(I-1),CAB(I-1))
          IF(ABS(CABPD).LT.EPSI) CABPD = EPSI

          XCT = X(I) + 0.5*DLT*(FN3(X(I),CAB(I)) + FN3(XSE,
*           CABPD))
          TSCT = TS(I) + 0.5*DLT*(FN4(TS(I),TG(I),X(I),CAB(I))
*           +FN4(TSSE,TGPD,XSE,CABPD))
          IF(ABS(XCT).LT.EPSI) XCT=EPSI
          CABCT = CAB(I-1) + 0.5*DLZ*(FN1(X(I-1),
*           CAB(I-1))+FN1(XCT,CABPD))
          IF(ABS(CABCT).LT.EPSI) CABCT = EPSI
          TGCT = TG(I-1)+0.5*DLZ*(FN2(TS(I-1),TG(I-1))
*           +FN2(TSCT,TGPD))

C

          X1(I) = X(I)
          TS1(I) = TS(I)
          CAB1(I) = CAB(I)
          TG1(I) = TG(I)
          X(I) = XCT
C      IF(X(I).GT.XRVNW(I)) X(I)=1.
          TS(I) = TSCT
          CAB(I) = CABCT
          TG(I) = TGCT

53      CONTINUE

C ----- COMPUTE AT: (i,j) = FROM (5,2) TO (INUM,2)

      DO 54 I = 5,INUM

          XSE = X(I)+DLT*FN3(X(I),CAB(I))
          TSSE = TS(I)+DLT*FN4(TS(I),TG(I),X(I),CAB(I))
          IF(ABS(XSE).LT.EPSI) XSE = EPSI

          TGPD = TG(I-1)+(DLZ/24.)*(55.*FN2(TS(I-1),TG(I-1))
*           -59.*FN2(TS(I-2),TG(I-2)) + 37.*FN2(TS(I-3),
*           TG(I-3))-9.*FN2(TS(I-4),TG(I-4)))
          CABPD = CAB(I-1)+(DLZ/24.)*(55.*FN1(X(I-1),CAB(I-1))

```

```

*      -59.*FN1(X(I-2),CAB(I-2)) + 37.*FN1(X(I-3),
*      CAB(I-3))-9.*FN1(X(I-4),CAB(I-4)))
IF(ABS(CABPD).LT.EPSI) CABPD = EPSI

XCT = X(I)+0.5*DLT*(FN3(X(I),CAB(I)) +
*      FN3(XSE,CABPD))
TSCT = TS(I)+0.5*DLT*(FN4(TS(I),TG(I),X(I),CAB(I))
*      +FN4(TSSE,TGPD,XSE,CABPD))
IF(ABS(XCT).LT.EPSI) XCT = EPSI

CABCT = CAB(I-1)+(DLZ/24.)*(9.*FN1(XCT,CABPD)
*      +19.*FN1(X(I-1),CAB(I-1)) - 5.*FN1(X(I-2),
*      CAB(I-2))+FN1(X(I-3),CAB(I-3)))
IF(ABS(CABCT).LT.EPSI) CABCT = EPSI
TGCT = TG(I-1)+(DLZ/24.)*(9.*FN2(TSCT,TGPD)
*      +19.*FN2(TS(I-1),TG(I-1)) - 5.*FN2(TS(I-2),
*      TG(I-2))+FN2(TS(I-3),TG(I-3)))

C
X1(I) = X(I)
TS1(I) = TS(I)
CAB1(I) = CAB(I)
TG1(I) = TG(I)

X(I) = XCT
C IF(X(I).GT.XRVNW(I)) X(I) = 1.
TS(I) = TSCT
CAB(I) = CABCT
TG(I) = TGCT

54 CONTINUE

C -----
C ----- GOING TO THE NEXT TIME STEP

T = T + DLT

C ----- COMPUTE AT: (i,j) = (1,3)

XPD = X1(1) + 2.0*DLT*FN3(X(1),CAB(1))
TSPD = TS1(1) + 2.0*DLT*FN4(TS(1),TG(1),X(1),CAB(1))
IF(ABS(XPD).LT.EPSI) XPD = EPSI
XCT = X(1)+0.5*DLT*(FN3(X(1),CAB(1))+FN3(XPD,CAB(1)))
TSCT = TS(1)+0.5*DLT*(FN4(TS(1),TG(1),X(1),CAB(1))
*      +FN4(TSPD,TG(1),XPD,CAB(1)))
IF(ABS(XCT).LT.EPSI) XCT=EPSI

X2(1) = X(1)
TS2(1) = TS(1)
X(1) = XCT
C IF(X(1).GT.XRVNW(1)) X(1) = 1.
TS(1) = TSCT

C ----- COMPUTE AT: (i,j) = (2,3)

```

```

CABSE = CAB(1) + DLZ*FN1(X(1),CAB(1))
IF(ABS(CABSE).LT.EPSI) CABSE = EPSI
TGSE = TG(1) + DLZ*FN2(TS(1),TG(1))
XPD = X1(2) + 2.0*DLT*FN3(X(2),CAB(2))
TSPD = TS1(2) + 2.0*DLT*FN4(TS(2),TG(2),X(2),CAB(2))
IF(ABS(XPD).LT.EPSI) XPD = EPSI
CABCT = CAB(1)+0.5*DLZ*(FN1(X(1),CAB(1))+FN1(
*      XPD,CABSE))
IF(ABS(CABCT).LT.EPSI) CABCT = EPSI
TGCT = TG(1) + 0.5*DLZ*(FN2(TS(1),TG(1))
*      + FN2(TSPD,TGSE))
XCT = X(2) + 0.5*DLT*(FN3(X(2),CAB(2))+
*      FN3(XPD,CABCT))
TSCT = TS(2)+0.5*DLT*(FN4(TS(2),TG(2),X(2),CAB(2))
*      +FN4(TSPD,TGCT,XPD,CABCT))
IF(ABS(XCT).LT.EPSI) XCT=EPSI

```

C

```

X2(2) = X(2)
TS2(2) = TS(2)
CAB2(2) = CAB(2)
TG2(2) = TG(2)

```

```

X(2) = XCT

```

C

```

IF(X(2).GT.XRVNW(2)) X(2)=1.
TS(2) = TSCT
CAB(2) = CABCT
TG(2) = TGCT

```

C ----- COMPUTE AT: (i,j) = (3,3) & (4,3)

```

DO 55 I = 3,4

```

```

CABPD = CAB(I-2)+2.0*DLZ*FN1(X(I-1),CAB(I-1))
IF(ABS(CABPD).LT.EPSI) CABPD = EPSI
TGPD = TG(I-2) + 2.0*DLZ*FN2(TS(I-1),TG(I-1))
XPD = X1(I) + 2.0*DLT*FN3(X(I),CAB(I))
IF(ABS(XPD).LT.EPSI) XPD=EPSI
TSPD = TS1(I) + 2.0*DLT*FN4(TS(I),TG(I),X(I),CAB(I))

CABCT = CAB(I-1)+0.5*DLZ*(FN1(X(I-1),
*      CAB(I-1))+FN1(XPD,CABPD))
IF(ABS(CABCT).LT.EPSI) CABCT = EPSI
TGCT = TG(I-1)+0.5*DLZ*(FN2(TS(I-1),TG(I-1))
*      +FN2(TSPD,TGPD))
XCT = X(I) + 0.5*DLT*(FN3(X(I),CAB(I))
*      + FN3(XPD,CABCT))
IF(ABS(XCT).LT.EPSI) XCT=EPSI
TSCT = TS(I) + 0.5*DLT*(FN4(TS(I),TG(I),X(I),CAB(I))
*      + FN4(TSPD,TGCT,XPD,CABCT))

```

C

```

X2(I) = X(I)
TS2(I) = TS(I)

```

```

CAB2(I) = CAB(I)
TG2(I) = TG(I)

X(I) = XCT
C   IF(X(I).GT.XRVNW(I)) X(I)=1.
TS(I) = TSCT
CAB(I) = CABCT
TG(I) = TGCT

55  CONTINUE

C ----- COMPUTE AT: (i,j) = FROM (5,3) TO (INUM,3)

DO 56 I=5,INUM

  CABPD = CAB(I-1)+(DLZ/24.)*(55.*FN1(X(I-1),CAB(I-1))
*   -59.*FN1(X(I-2),CAB(I-2))+37.*FN1(X(I-3),
*   CAB(I-3))-9.*FN1(X(I-4),CAB(I-4)))
  IF(ABS(CABPD).LT.EPSI) CABPD = EPSI
  TGPD = TG(I-1)+(DLZ/24.)*(55.*FN2(TS(I-1),TG(I-1))
*   -59.*FN2(TS(I-2),TG(I-2))+37.*FN2(TS(I-3),
*   TG(I-3))-9.*FN2(TS(I-4),TG(I-4)))
  XPD = X1(I)+2.0*DLT*FN3(X(I),CAB(I))
  IF(ABS(XPD).LT.EPSI) XPD = EPSI
  TSPD = TS1(I)+2.0*DLT*FN4(TS(I),TG(I),X(I),CAB(I))

  CABCT = CAB(I-1)+(DLZ/24.)*(9.*FN1(XPD,CABPD)
*   +19.*FN1(X(I-1),CAB(I-1))-5.*FN1(X(I-2),
*   CAB(I-2))+FN1(X(I-3),CAB(I-3)))
  IF(ABS(CABCT).LT.EPSI) CABCT = EPSI
  TGCT = TG(I-1)+(DLZ/24.)*(9.*FN2(TSPD,TGPD)
*   +19.*FN2(TS(I-1),TG(I-1))
*   -5.*FN2(TS(I-2),TG(I-2))+FN2(TS(I-3),TG(I-3)))
  XCT = X(I)+0.5*DLT*(FN3(X(I),CAB(I))+FN3(XPD,CABCT))
  IF(ABS(XCT).LT.EPSI) XCT = EPSI
  TSCT = TS(I)+0.5*DLT*(FN4(TS(I),TG(I),X(I),CAB(I))
*   +FN4(TSPD,TGCT,XPD,CABCT))

C

X2(I)=X(I)
TS2(I)=TS(I)
CAB2(I) = CAB(I)
TG2(I) = TG(I)

X(I)= XCT
C   IF(X(I).GT.XRVNW(I)) X(I)=1.
TS(I)= TSCT
CAB(I)= CABCT
TG(I)= TGCT

56  CONTINUE

C -----
C ----- GOING TO THE NEXT TIME STEP

```

T = T + DLT

C ----- COMPUTE AT: (i,j) = (1,4)

```

XPD = X2(1) + 2.0*DLT*FN3(X(1),CAB(1))
TSPD = TS2(1) + 2.0*DLT*FN4(TS(1),TG(1),X(1),CAB(1))
IF(ABS(XPD).LT.EPSI) XPD = EPSI
XCT = X(1) + 0.5*DLT*(FN3(X(1),CAB(1))+
*      FN3(XPD,CAB(1)))
TSCT = TS(1) + 0.5*DLT*(FN4(TS(1),TG(1),X(1),CAB(1))
*      +FN4(TSPD,TG(1),XPD,CAB(1)))
IF(ABS(XCT).LT.EPSI) XCT = EPSI

```

C

```

X3(1) = X(1)
TS3(1) = TS(1)
X(1) = XCT

```

C IF(X(1).GT.XRVNW(1)) X(1) = 1.
 TS(1) = TSCT

C ----- COMPUTE AT: (i,j) = (2,4)

```

CABSE = CAB(1) + DLZ*FN1(X(1),CAB(1))
IF(ABS(CABSE).LT.EPSI) CABSE = EPSI
TGSE = TG(1) + DLZ*FN2(TS(1),TG(1))
XPD = X2(2) + 2.0*DLT*FN3(X(2),CAB(2))
TSPD = TS2(2) + 2.0*DLT*FN4(TS(2),TG(2),X(2),CAB(2))
IF(ABS(XPD).LT.EPSI) XPD = EPSI

```

```

CABCT = CAB(1) + 0.5*DLZ*(FN1(X(1),CAB(1)) +
*      FN1(XPD,CABSE))
IF(ABS(CABCT).LT.EPSI) CABCT = EPSI
TGCT =TG(1)+0.5*DLZ*(FN2(TS(1),TG(1))+FN2(TSPD,TGSE))
XCT = X(2) +0.5*DLT*(FN3(X(2),CAB(2))+FN3(XPD,CABCT))
TSCT = TS(2) + 0.5*DLT*(FN4(TS(2),TG(2),X(2),CAB(2))
*      +FN4(TSPD,TGCT,XPD,CABCT))
IF(ABS(XCT).LT.EPSI) XCT = EPSI

```

C

```

X3(2) = X(2)
TS3(2) = TS(2)
CAB3(2) = CAB(2)
TG3(2) = TG(2)

```

C X(2) = XCT
 IF(X(2).GT.XRVNW(2)) X(2)=1.
 TS(2) = TSCT
 CAB(2) = CABCT
 TG(2) = TGCT

C ----- COMPUTE AT: (i,j) = (3,4) & (4,4)

DO 57 I = 3,4

```

CABPD = CAB(I-2)+2.0*DLZ*FN1(X(I-1),CAB(I-1))

```



```

IF(ABS(CABPD).LT.EPSI) CABPD = EPSI
TGPD = TG(I-2) + 2.0*DLZ*FN2(TS(I-1),TG(I-1))
XPD = X2(I) + 2.0*DLT*FN3(X(I),CAB(I))
IF(ABS(XPD).LT.EPSI) XPD = EPSI
TSPD = TS2(I) + 2.0*DLT*FN4(TS(I),TG(I),X(I),CAB(I))

```

```

CABCT = CAB(I-1)+0.5*DLZ*(FN1(X(I-1),CAB(I-1))+
*      FN1(XPD,CABPD))
IF(ABS(CABCT).LT.EPSI) CABCT = EPSI
TGCT = TG(I-1)+0.5*DLZ*(FN2(TS(I-1),TG(I-1))+
*      FN2(TSPD,TGPD))
XCT = X(I)+0.5*DLT*(FN3(X(I),CAB(I))+FN3(XPD,CABCT))
IF(ABS(XCT).LT.EPSI) XCT =EPSI
TSCT = TS(I)+0.5*DLT*(FN4(TS(I),TG(I),X(I),CAB(I))
*      + FN4(TSPD,TGCT,XPD,CABCT))

```

C

```

X3(I) = X(I)
TS3(I) = TS(I)
CAB3(I) = CAB(I)
TG3(I) = TG(I)

```

C

```

X(I) = XCT
IF(X(I).GT.XRVNW(I)) X(I) = 1.
TS(I) = TSCT
CAB(I) = CABCT
TG(I) = TGCT

```

57 CONTINUE

C ----- COMPUTE AT: (i,j) = FROM (5,4) TO (INUM,4)

DO 58 I = 5,INUM

```

CABPD = CAB(I-1)+(DLZ/24.)*(55.*FN1(X(I-1),CAB(I-1))
*      -59.*FN1(X(I-2),CAB(I-2))+37.*FN1(X(I-3),
*      CAB(I-3))-9.*FN1(X(I-4),CAB(I-4)))
IF(ABS(CABPD).LT.EPSI) CABPD = EPSI
TGPD = TG(I-1)+(DLZ/24.)*(55.*FN2(TS(I-1),TG(I-1))
*      -59.*FN2(TS(I-2),TG(I-2))+37.*FN2(TS(I-3),
*      TG(I-3))-9.*FN2(TS(I-4),TG(I-4)))
XPD = X2(I)+2.0*DLT*FN3(X(I),CAB(I))
IF(ABS(XPD).LT.EPSI) XPD=EPSI
TSPD = TS2(I)+2.0*DLT*FN4(TS(I),TG(I),X(I),CAB(I))

CABCT = CAB(I-1)+(DLZ/24.)*(9.*FN1(XPD,CABPD)
*      +19.*FN1(X(I-1),CAB(I-1))
*      -5.*FN1(X(I-2),CAB(I-2))+FN1(X(I-3),CAB(I-3)))
IF(ABS(CABCT).LT.EPSI) CABCT = EPSI
TGCT = TG(I-1)+(DLZ/24.)*(9.*FN2(TSPD,TGPD)
*      +19.*FN2(TS(I-1),TG(I-1))
*      -5.*FN2(TS(I-2),TG(I-2))+FN2(TS(I-3),TG(I-3)))
XCT = X(I)+0.5*DLT*(FN3(X(I),CAB(I))+FN3(XPD,CABCT))
IF(ABS(XCT).LT.EPSI) XCT = EPSI
TSCT = TS(I)+0.5*DLT*(FN4(TS(I),TG(I),X(I),CAB(I))

```

```

*      +FN4(TSPD,TGCT,XPD,CABCT))

C
  X3(I) = X(I)
  TS3(I) = TS(I)
  CAB3(I) = CAB(I)
  TG3(I) = TG(I)

  X(I) = XCT
C   IF(X(I).GT.XRVNW(I)) X(I) = 1.
  TS(I) = TSCT
  CAB(I) = CABCT
  TG(I) = TGCT

58  CONTINUE

C -----
C ----- GOING TO THE NEXT TIME STEP

      T = T + DLT

C ----- COMPUTE UP TO THE FINAL TIME STEP
C
  JSTP = INT(TEND/DLT) + 2
  I1 = 0
  I5 = 2
  DO 100 J = 5,JSTP

C ----- COMPUTE AT: i = 1

  XPD = X(1)+(DLT/24.)*(55.*FN3(X(1),CAB(1))
*   -59.*FN3(X3(1),CAB(1))+37.*FN3(X2(1),CAB(1))
*   -9.*FN3(X1(1),CAB(1)))
  TSPD = TS(1)+(DLT/24.)*(55.*FN4(TS(1),TG(1),X(1),
*   CAB(1))-59.*FN4(TS3(1),TG(1),X3(1),CAB(1))
*   +37.*FN4(TS2(1),TG(1),X2(1),CAB(1))
*   -9.*FN4(TS1(1),TG(1),X1(1),CAB(1)))
  IF(ABS(XPD).LT.EPSI) XPD=EPSI

  XCT = X(1)+(DLT/24.)*(9.*FN3(XPD,CAB(1))+19.*
*   FN3(X(1),CAB(1))-5.*FN3(X3(1),CAB(1))+
*   FN3(X2(1),CAB(1)))
  TSCT = TS(1)+(DLT/24.)*(9.*FN4(TSPD,TG(1),XPD,CAB(1))
*   +19.*FN4(TS(1),TG(1),X(1),CAB(1))
*   -5.*FN4(TS3(1),TG(1),X3(1),
*   CAB(1))+FN4(TS2(1),TG(1),X2(1),CAB(1)))
  IF(ABS(XCT).LT.EPSI) XCT = EPSI

C
  X1(1) = X2(1)
  X2(1) = X3(1)
  TS1(1) = TS2(1)
  TS2(1) = TS3(1)

  X3(1) = X(1)

```

```

TS3(1) = TS(1)
X(1) = XCT
C   IF(X(1).GT.XRVNW(1)) X(1) = 1.
TS(1) = TSCT

C ----- COMPUTE AT: i = 2

CABSE = CAB(1)+DLZ*FN1(X(1),CAB(1))
IF(ABS(CABSE).LT.EPSI) CABSE=EPSI
TGSE = TG(1)+DLZ*FN2(TS(1),TG(1))
XPD = X(2)+(DLT/24.)*(55.*FN3(X(2),CAB(2))
*   -59.*FN3(X3(2),CAB3(2))
*   +37.*FN3(X2(2),CAB2(2))-9.*FN3(X1(2),CAB1(2)))
TSPD = TS(2)+(DLT/24.)*(55.*FN4(TS(2),TG(2),X(2),
*   CAB(2))-59.*FN4(TS3(2),TG3(2),X3(2),CAB3(2))
*   +37.*FN4(TS2(2),TG2(2),X2(2),CAB2(2))-9.*
*   FN4(TS1(2),TG1(2),X1(2),CAB1(2)))
IF(ABS(XPD).LT.EPSI) XPD = EPSI

CABCT = CAB(1)+0.5*DLZ*(FN1(X(1),CAB(1))+
*   FN1(XPD,CABSE))
IF(ABS(CABCT).LT.EPSI) CABCT = EPSI
TGCT =TG(1)+0.5*DLZ*(FN2(TS(1),TG(1))+FN2(TSPD,TGSE))
XCT = X(2)+(DLT/24.)*(9.*FN3(XPD,CABCT)+19.*FN3(X(2),
*   CAB(2))-5.*FN3(X3(2),CAB3(2))+FN3(X2(2),CAB2(2)))
TSCT = TS(2)+(DLT/24.)*(9.*FN4(TSPD,TGCT,XPD,CABCT)
*   +19.*FN4(TS(2),TG(2),X(2),CAB(2))
*   -5.*FN4(TS3(2),TG3(2),X3(2),CAB3(2))
*   +FN4(TS2(2),TG2(2),X2(2),CAB2(2)))
IF(ABS(XCT).LT.EPSI) XCT = EPSI

C

X1(2) = X2(2)
X2(2) = X3(2)
TS1(2) = TS2(2)
TS2(2) = TS3(2)
CAB1(2) = CAB2(2)
CAB2(2) = CAB3(2)
TG1(2) = TG2(2)
TG2(2) = TG3(2)

X3(2) = X(2)
TS3(2) = TS(2)
CAB3(2) = CAB(2)
TG3(2) = TG(2)

X(2) = XCT
C   IF(X(2).GT.XRVNW(2)) X(2) =1.
TS(2) = TSCT
CAB(2) = CABCT
TG(2) = TGCT

C ----- COMPUTE AT: i = 3 & 4

DO 60 I = 3,4

```

```

CABPD = CAB(I-2)+2.*DLZ*FN1(X(I-1),CAB(I-1))
IF(ABS(CABPD).LT.EPSI) CABPD = EPSI
TGPD = TG(I-2)+2.*DLZ*FN2(TS(I-1),TG(I-1))
XPD = X(I)+(DLT/24.)*(55.*FN3(X(I),CAB(I))
*      -59.*FN3(X3(I),CAB3(I))
*      +37.*FN3(X2(I),CAB2(I))-9.*FN3(X1(I),CAB1(I)))
TSPD = TS(I)+(DLT/24.)*(55.*FN4(TS(I),TG(I),X(I),
*      CAB(I))-59.*FN4(TS3(I),TG3(I),X3(I),CAB3(I))
*      +37.*FN4(TS2(I),TG2(I),X2(I),CAB2(I))-9.*
*      FN4(TS1(I),TG1(I),X1(I),CAB1(I)))
IF(ABS(XPD).LT.EPSI) XPD = EPSI

CABCT = CAB(I-1)+0.5*DLZ*(FN1(X(I-1),CAB(I-1))+
*      FN1(XPD,CABPD))
IF(ABS(CABCT).LT.EPSI) CABCT = EPSI
TGCT = TG(I-1)+0.5*DLZ*(FN2(TS(I-1),TG(I-1))+
*      FN2(TSPD,TGPD))
XCT = X(I)+(DLT/24.)*(9.*FN3(XPD,CABCT)+19.*
*      FN3(X(I),CAB(I))-5.*FN3(X3(I),CAB3(I))+
*      FN3(X2(I),CAB2(I)))
IF(ABS(XCT).LT.EPSI) XCT = EPSI
TSCT = TS(I)+(DLT/24.)*(9.*FN4(TSPD,TGCT,XPD,CABCT)
*      +19.*FN4(TS(I),TG(I),X(I),CAB(I))
*      -5.*FN4(TS3(I),TG3(I),X3(I),CAB3(I))
*      +FN4(TS2(I),TG2(I),X2(I),CAB2(I)))

```

C

```

X1(I) = X2(I)
X2(I) = X3(I)
TS1(I) = TS2(I)
TS2(I) = TS3(I)
CAB1(I) = CAB2(I)
CAB2(I) = CAB3(I)
TG1(I) = TG2(I)
TG2(I) = TG3(I)

```

```

X3(I) = X(I)
TS3(I) = TS(I)
CAB3(I) = CAB(I)
TG3(I) = TG(I)

```

```

X(I) = XCT

```

```

C IF(X(I).GT.XRVNW(I)) X(I)=1.
TS(I) = TSCT
CAB(I) = CABCT
TG(I) = TGCT

```

60 CONTINUE

C ----- COMPUTE AT: i = FROM 5 TO INUM

```

DO 62 I = 5, INUM

```

```

CABPD = CAB(I-1)+(DLZ/24.)*(55.*FN1(X(I-1),CAB(I-1))

```

```

*      -59.*FN1(X(I-2),CAB(I-2))+37.*FN1(X(I-3),
*      CAB(I-3))-9.*FN1(X(I-4),CAB(I-4))
IF(ABS(CABPD).LT.EPSI) CABPD= EPSI
TGPD = TG(I-1)+(DLZ/24.)*(55.*FN2(TS(I-1),TG(I-1))
*      -59.*FN2(TS(I-2),TG(I-2))+37.*FN2(TS(I-3),
*      TG(I-3))-9.*FN2(TS(I-4),TG(I-4)))
XPD = X(I)+(DLT/24.)*(55.*FN3(X(I),CAB(I))
*      -59.*FN3(X3(I),CAB3(I))
*      +37.*FN3(X2(I),CAB2(I))-9.*FN3(X1(I),CAB1(I)))
TSPD = TS(I)+(DLT/24.)*(55.*FN4(TS(I),TG(I),X(I),
*      CAB(I))-59.*FN4(TS3(I),TG3(I),X3(I),CAB3(I))
*      +37.*FN4(TS2(I),TG2(I),X2(I),CAB2(I))
*      -9.*FN4(TS1(I),TG1(I),X1(I),CAB1(I)))
IF(ABS(XPD).LT.EPSI) XPD = EPSI

```

C ----- NUMBER OF CORRECTION

NCRT = 2

DO 666 K = 1,NCRT

```

CABCT = CAB(I-1)+(DLZ/24.)*(9.*FN1(XPD,CABPD)
*      +19.*FN1(X(I-1),CAB(I-1))
*      -5.*FN1(X(I-2),CAB(I-2))+FN1(X(I-3),CAB(I-3)))
IF(ABS(CABCT).LT.EPSI) CABCT = EPSI
TGCT = TG(I-1)+(DLZ/24.)*(9.*FN2(TSPD,TGPD)
*      +19.*FN2(TS(I-1),TG(I-1))
*      -5.*FN2(TS(I-2),TG(I-2))+FN2(TS(I-3),TG(I-3)))
XCT = X(I)+(DLT/24.)*(9.*FN3(XPD,CABCT)+19.*
*      FN3(X(I),CAB(I))-5.*FN3(X3(I),CAB3(I))+
*      FN3(X2(I),CAB2(I)))
IF(ABS(XCT).LT.EPSI) XCT = EPSI
TSCT = TS(I)+(DLT/24.)*(9.*FN4(TSPD,TGCT,XPD,CABCT)
*      +19.*FN4(TS(I),TG(I),X(I),CAB(I))
*      -5.*FN4(TS3(I),TG3(I),X3(I),CAB3(I))
*      +FN4(TS2(I),TG2(I),X2(I),CAB2(I)))

```

C

```

CABPD = CABCT
XPD = XCT
TGPD = TGCT
TSPD = TSCT

```

666 CONTINUE

C

```

X1(I) = X2(I)
X2(I) = X3(I)
TS1(I) = TS2(I)
TS2(I) = TS3(I)
CAB1(I) = CAB2(I)
CAB2(I) = CAB3(I)
TG1(I) = TG2(I)
TG2(I) = TG3(I)

```

```

X3(I) = X(I)
TS3(I) = TS(I)
CAB3(I) = CAB(I)
TG3(I) = TG(I)

```

```

X(I) = XCT
TS(I) = TSCT
CAB(I) = CABCT
TG(I) = TGCT

```

```
62 CONTINUE
```

```

C -----
C ----- GOING TO THE NEXT TIME STEP

```

```
T = T + DLT
```

```
C -----
```

```

IF((.NOT.BKTIME).AND.(CAB(INUM)*CABPPM.GE.BKPPM)) THEN
  TIMEBK = T

```

```

DO 69 I = 1, INUM
  BKSX(I) = X(I)

```

```
69 CONTINUE
```

```

BKTIME = .TRUE.
END IF

```

```
C -----
```

```

IF((TINT*10.).GE.1.) FACT = 10
IF((TINT*10.).GE.10.) FACT = 1
JBGIN = INT(TBGIN*FACT*1.001)
JINT = INT(TINT*FACT*1.001)
JEND = INT(TEND*FACT*1.001)

```

```
DO 72 JJ = JBGIN, JEND, JINT
```

```

IF(ABS(T-JJ/FACT).LT.EPS) THEN
  WRITE (6,400) T

```

```

DO 77 INO = 1, INUM
  SULTG(I1+INO) = TG(INO)
  SULTS(I1+INO) = TS(INO)
  SULCAB(I1+INO) = CAB(INO)
  SULX(I1+INO) = X(INO)
  SULOAD(I1+INO) = TSLOAD/(X(INO)+81.38/97.44*
    (1.-X(INO)))*X(INO)

```

```
77 * CONTINUE
```

```
I1 = I1 + INUM
```

```

PPMEXT(I5) = CAB(INUM)*CABPPM
I5 = I5 + 1

```

```

                END IF

72      CONTINUE

C ----- FOR TEMP. VS TIME

        DO 81 JT = 1, NTIME

                IF (ABS(T-BTBGIN*JT).LE.EPS) THEN

                        DO 83 NL = 1, NBLIN
                                TGIMSI(NL,NT) = TG(IBPNT(NL))
                                TSIMSI(NL,NT) = TS(IBPNT(NL))
83
                                NT = NT + 1

                        END IF

81      CONTINUE

C -----

100     CONTINUE

C -----

        IF(BKTIME) THEN
                OPEN(14,FILE='HBKX11')
                OPEN(18,FILE='HAVX11')
C
                WRITE(6,101) TIMEBK
101     FORMAT(//' BREAKTHROUGH TIME = ',F8.2, 'hr')

                DO 103 I = 1, INUM
                        WRITE (14,122) BKSX(I)
103     FORMAT(E14.4)

                SUMX = 0.0
                DO 107 I = 1, INUM
                        SUMX = SUMX + BKSX(I)
107     CONTINUE
                AVEX = SUMX/INUM

                WRITE(18,133) AVEX
133     FORMAT(//' AVERAGE X AT BREAKTHROUGH = ',F10.4)
                CLOSE(14)
                CLOSE(18)

        ELSE

                WRITE(6,102)
102     FORMAT(//' TIMEBK EXCEEDS ENDING TIME !!')

```

```

      END IF

C ----- FOR TEMP. VS TIME

      NLA = 0

      DO 85 L = 1, NBLIN

          DO 87 M = 1, NT-1

              BTG(NLA+M) = TGIMSI(L,M)
87              BTS(NLA+M) = TSIMSI(L,M)

              NLA = NLA + NT-1

85      CONTINUE

C ----- PRINT SIMULATION RESULTS

      NTLIN = INT((TEND-TBGIN)/TINT*1.001) + 1

      CALL PPMOUT(PPMEXT,NTLIN,TBGIN,TINT)
      CALL OUTPUT(SULCAB,SULX,SULOAD,SULTG,SULTS,NTLIN,
*               TBGIN,TINT)
      CALL TMOU(TBGIN,BINT,NBLIN,BTBGIN,BTG,BTS)

C      RETURN

400  FORMAT(/'          INTEGRATED TO ',F9.2,' hr')
      RETURN
      END

C ----- END OF SUBROUTINE AMPC

C -----

C ----- SUBROUTINE PPMOUT

      SUBROUTINE PPMOUT(PPMEXT,NTLIN,TBGIN,TINT)
      DIMENSION PPMEXT(12550)
      OPEN(11,FILE='HPM11.DAT',STATUS='NEW')

      WRITE(11,999)
999  FORMAT(///'          TIME(hr)'
*         '          EXIT H2S(ppm) '///)
      DO 491 I = 2,NTLIN+1
      WRITE(11,888) TBGIN+TINT*(I-2), PPMEXT(I)
491  CONTINUE

888  FORMAT(16X,F8.2,10X,E10.3)

      CLOSE(11)

```



```

RETURN
END

```

C ----- SUBROUTINE OUTPUT

```

SUBROUTINE OUTPUT(SULCAB,SULX,SULOAD,SULTG,SULTS,
*
*           NTLIN,TBGIN,TINT)
DIMENSION Z(51)
DIMENSION SULCAB(12550),SULX(12550),SULOAD(12550),
*
*           SULTG(12550),SULTS(12550)
COMMON /COM1/ INUM
OPEN(12,FILE='HSL11.DAT',STATUS='NEW')

I1 = 1

DO 91 I = 1,51
91   Z(I) = 0. + (I-1)*0.02

DO 95 I = 1,NTLIN
    WRITE(12,97) TBGIN + TINT*(I-1)

    DO 94 I2 = 1,51
        I3 = I1 + (INUM-1)/50*(I2-1)
94   WRITE(12,98) Z(I2), SULCAB(I3),SULX(I3),SULOAD(I3),
*
*           SULTG(I3),SULTS(I3)

        I1=I1+INUM

95   CONTINUE

97   FORMAT(//'
*   TIME ='
*,F8.3,      ' (hr) >>'
*//'
*           (Z)      (CAB)      (X)      (SL)'
*           '      (TG)      (TS)'
*/)

98   FORMAT(12X,F5.3,1X,E10.4,1X,E10.4,1X,E10.4,1X,
*
*           E10.4,1X,E10.4/)

CLOSE(12)
RETURN
END

```

C ----- SUBROUTINE TMPOUT

```

SUBROUTINE TMPOUT(BBGIN,BINT,NBLIN,BTBGIN,BTG,BTS)
DIMENSION TIME(51)
DIMENSION BTG(500), BTS(500)
COMMON /COM1/ INUM
OPEN(13,FILE='HTP11.DAT',STATUS='NEW')

NTIME = 50
K2 = 0

```

```

DO 222 K = 1, NTIME
222  TIME(K) = 0. + K*BTBGIN

DO 223 K1 = 1, NBLIN
    WRITE(13,229) BBDIN+BINT*(K1-1)

    DO 88 K3 = 1, NTIME
        K2 = K2 + 1
        WRITE(13,77) TIME(K3), BTG(K2), BTS(K2)
88      CONTINUE

223  CONTINUE

229  FORMAT(//'                                << AT BED LOCATION = '
*      ,F8.3,' >>'
*      //'
*      '                                TIME          GAS TEMP'
*      '                                SORBENT TEMP'
*      /'                                (HR)          (TG)'
*      '                                (TS)'
*/)
77      FORMAT(11X,F9.4,5X,E11.4,5X,E11.4)

CLOSE(13)
RETURN
END

C -----
C ----- FUNCTION FN1

FUNCTION FN1(X,CAB)
FN1 = -CAB*BETA(X)
RETURN
END

C ----- FUNCTION FN2

FUNCTION FN2(TS,TG)
COMMON /COM2/ FC2
FN2 = FC2*(TS-TG)
RETURN
END

C ----- FUNCTION FN3

FUNCTION FN3(X,CAB)
COMMON /COM3/ FC1
FN3 = FC1*BETA(X)*CAB
RETURN
END

C ----- FUNCTION FN4

FUNCTION FN4(TS,TG,X,CAB)
COMMON /COM4/ FC3,FC4

```

```
FN4 = FC3*RBV(X,CAB)-FC4*(TS-TG)
RETURN
END
```

```
C ----- FUNCTION RBV
```

```
FUNCTION RBV(X,CAB)
COMMON /COM6/ FCRBV
RBV = FCRBV*BETA(X)*CAB
RETURN
END
```

```
C ----- FUNCTION BETA
```

```
FUNCTION BETA(X)
COMMON /COM7/ FCBTA1,FCBTA3,FCBTA2,DE1,R
IF(X.LT.1.) GO TO 201
BETA = 0.
RETURN
```

```
201 BETA = FCBTA1/(FCBTA2 + (1./((1.-X)**0.5))*FCBTA3
*      -(0.5*R**2/DE1)*LOG(1.-X))
```

```
RETURN
END
```

APPENDIX C

OUTPUT FROM SULFIDATION SIMULATION

The following are obtained from the sulfidation simulation:

- 1) Sorbent conversion at breakthrough time, (Value at each grid point along the reactor axis is shown.)
- 2) Average sorbent conversion in the reactor at breakthrough time,
- 3) Sulfidation time vs exit H_2S concentration,
- 4) Values of H_2S concentration, sorbent conversion, sulfur loading, gas temperature and sorbent temperature along the reactor at specified times, and
- 5) Values of gas temperature and sorbent temperature along the time axis at specified bed locations

Section 1

	x		x		x		x
i=1	.1000E+01	i=41	.1000E+01	i=81	.1000E+01	i=121	.9982E+00
	.1000E+01		.1000E+01		.1000E+01		.9958E+00
	.1000E+01		.1000E+01		.1000E+01		.9931E+00
	.1000E+01		.1000E+01		.1000E+01		.9902E+00
	.1000E+01		.1000E+01		.1000E+01		.9870E+00
	.1000E+01		.1000E+01		.1000E+01		.9838E+00
	.1000E+01		.1000E+01		.1000E+01		.9803E+00
	.1000E+01		.1000E+01		.1000E+01		.9767E+00
	.1000E+01		.1000E+01		.1000E+01		.9730E+00
	.1000E+01		.1000E+01		.1000E+01		.9691E+00
	.1000E+01		.1000E+01		.1000E+01		.9651E+00
	.1000E+01		.1000E+01		.1000E+01		.9610E+00
	.1000E+01		.1000E+01		.1000E+01		.9568E+00
	.1000E+01		.1000E+01		.1000E+01		.9524E+00
	.1000E+01		.1000E+01		.1000E+01		.9480E+00
	.1000E+01		.1000E+01		.1000E+01		.9434E+00
	.1000E+01		.1000E+01		.1000E+01		.9387E+00
	.1000E+01		.1000E+01		.1000E+01		.9339E+00
	.1000E+01		.1000E+01		.1000E+01		.9290E+00
	.1000E+01		.1000E+01		.1000E+01		.9240E+00
	.1000E+01		.1000E+01		.1000E+01		.9190E+00
	.1000E+01		.1000E+01		.1000E+01		.9138E+00
	.1000E+01		.1000E+01		.1000E+01		.9085E+00
	.1000E+01		.1000E+01		.1000E+01		.9031E+00
	.1000E+01		.1000E+01		.1000E+01		.8976E+00
	.1000E+01		.1000E+01		.1000E+01		.8920E+00
	.1000E+01		.1000E+01		.1000E+01		.8864E+00
	.1000E+01		.1000E+01		.1000E+01		.8806E+00
	.1000E+01		.1000E+01		.1000E+01		.8748E+00
	.1000E+01		.1000E+01		.1000E+01		.8688E+00
	.1000E+01		.1000E+01		.1000E+01		.8628E+00
	.1000E+01		.1000E+01		.1000E+01		.8566E+00
	.1000E+01		.1000E+01		.1000E+01		.8504E+00
	.1000E+01		.1000E+01		.1000E+01		.8441E+00
	.1000E+01		.1000E+01		.1000E+01		.8377E+00
	.1000E+01		.1000E+01		.1000E+01		.8312E+00
	.1000E+01		.1000E+01		.1000E+01		.8247E+00
	.1000E+01		.1000E+01		.1000E+01		.8180E+00
	.1000E+01		.1000E+01		.1000E+01		.8113E+00
	.1000E+01		.1000E+01		.1000E+01		.8044E+00

i=161	.7975E+00	i=184	.6152E+00	i=207	.3919E+00	i=230	.1411E+00
	.7905E+00		.6063E+00		.3813E+00		.1304E+00
	.7834E+00		.5974E+00		.3708E+00		.1198E+00
	.7762E+00		.5883E+00		.3601E+00		.1094E+00
	.7690E+00		.5792E+00		.3494E+00		.9911E-01
	.7616E+00		.5700E+00		.3387E+00		.8905E-01
	.7542E+00		.5607E+00		.3279E+00		.7926E-01
	.7467E+00		.5513E+00		.3170E+00		.6978E-01
	.7391E+00		.5419E+00		.3062E+00		.6067E-01
	.7314E+00		.5324E+00		.2952E+00		.5200E-01
	.7236E+00		.5228E+00		.2843E+00		.4384E-01
	.7158E+00		.5132E+00		.2733E+00		.3628E-01
	.7078E+00		.5034E+00		.2623E+00		.2940E-01
	.6998E+00		.4936E+00		.2512E+00		.2328E-01
	.6917E+00		.4838E+00		.2402E+00		.1799E-01
	.6836E+00		.4738E+00		.2291E+00		.1355E-01
	.6753E+00		.4638E+00		.2180E+00		.9959E-02
	.6670E+00		.4537E+00		.2069E+00		.7151E-02
	.6585E+00		.4436E+00		.1959E+00		.5033E-02
	.6500E+00		.4334E+00		.1848E+00		.3483E-02
	.6415E+00		.4231E+00		.1738E+00		.2380E-02
	.6328E+00		.4127E+00		.1629E+00		.1610E-02
	.6241E+00		.4023E+00		.1520E+00		

Section 2

AVERAGE X AT BREAKTHROUGH = .7657

Section 3

TIME(HR)	EXIT H ₂ S(PPM)
.40	.185E-34
.80	.108E-31
1.20	.173E-29
1.60	.145E-27
2.00	.814E-26
2.40	.347E-24
2.80	.121E-22
3.20	.369E-21
3.60	.102E-19
4.00	.276E-18
4.40	.749E-17
4.80	.203E-15
5.20	.551E-14
5.60	.150E-12
6.00	.406E-11
6.40	.110E-09
6.80	.299E-08
7.20	.810E-07
7.60	.220E-05
8.00	.596E-04
8.40	.162E-02
8.80	.439E-01
9.20	.119E+01
9.60	.308E+02
10.00	.441E+03
10.40	.168E+04
10.80	.327E+04
11.20	.493E+04
11.60	.657E+04
12.00	.815E+04
12.40	.964E+04
12.80	.111E+05
13.20	.124E+05
13.60	.136E+05
14.00	.147E+05
14.40	.157E+05
14.80	.166E+05
15.20	.174E+05
15.60	.181E+05

16.00	.187E+05
16.40	.188E+05
16.80	.188E+05
17.20	.188E+05
17.60	.188E+05
18.00	.188E+05
18.40	.188E+05
18.80	.188E+05
19.20	.188E+05
19.60	.188E+05
20.00	.188E+05

Section 4

<< AT SULFIDATION TIME = 1.000 (hr) >>

(Z)	(CAB)	(X)	(SL)	(TG)	(TS)
.000	.1000E+01	.6307E+00	.2205E+00	.1000E+01	.1002E+01
.040	.8556E+00	.5396E+00	.1918E+00	.1005E+01	.1007E+01
.080	.6994E+00	.4411E+00	.1596E+00	.1010E+01	.1012E+01
.120	.5328E+00	.3361E+00	.1239E+00	.1016E+01	.1018E+01
.160	.3590E+00	.2264E+00	.8521E-01	.1022E+01	.1025E+01
.200	.1859E+00	.1173E+00	.4507E-01	.1028E+01	.1031E+01
.240	.4415E-01	.2784E-01	.1089E-01	.1034E+01	.1035E+01
.280	.1557E-02	.9814E-03	.3858E-03	.1035E+01	.1035E+01
.320	.2572E-04	.1621E-04	.6374E-05	.1035E+01	.1035E+01
.360	.4131E-06	.2604E-06	.1024E-06	.1035E+01	.1035E+01
.400	.6635E-08	.4182E-08	.1644E-08	.1035E+01	.1035E+01
.440	.1065E-09	.6716E-10	.2641E-10	.1035E+01	.1035E+01
.480	.1711E-11	.1078E-11	.4241E-12	.1035E+01	.1035E+01
.520	.2748E-13	.1732E-13	.6810E-14	.1035E+01	.1035E+01
.560	.4412E-15	.2781E-15	.1094E-15	.1035E+01	.1035E+01
.600	.7085E-17	.4466E-17	.1756E-17	.1035E+01	.1035E+01
.640	.1138E-18	.7172E-19	.2820E-19	.1035E+01	.1035E+01
.680	.1827E-20	.1152E-20	.4529E-21	.1035E+01	.1035E+01
.720	.2934E-22	.1850E-22	.7273E-23	.1035E+01	.1035E+01
.760	.4712E-24	.2970E-24	.1168E-24	.1035E+01	.1035E+01
.800	.7567E-26	.4770E-26	.1876E-26	.1036E+01	.1036E+01
.840	.1215E-27	.7660E-28	.3012E-28	.1036E+01	.1036E+01
.880	.1951E-29	.1230E-29	.4837E-30	.1036E+01	.1036E+01

.920	.3134E-31	.1975E-31	.7767E-32	.1036E+01	.1036E+01
.960	.5032E-33	.3172E-33	.1247E-33	.1036E+01	.1036E+01
1.000	.8081E-35	.5094E-35	.2003E-35	.1036E+01	.1036E+01

<< AT SULFIDATION TIME = 2.000 (hr) >>

(Z)	(CAB)	(X)	(SL)	(TG)	(TS)
.000	.1000E+01	.8364E+00	.2823E+00	.1000E+01	.1001E+01
.040	.9176E+00	.7675E+00	.2621E+00	.1003E+01	.1004E+01
.080	.8250E+00	.6901E+00	.2388E+00	.1006E+01	.1007E+01
.120	.7228E+00	.6045E+00	.2124E+00	.1009E+01	.1011E+01
.160	.6112E+00	.5112E+00	.1826E+00	.1013E+01	.1015E+01
.200	.4909E+00	.4106E+00	.1494E+00	.1017E+01	.1019E+01
.240	.3634E+00	.3039E+00	.1127E+00	.1022E+01	.1024E+01
.280	.2315E+00	.1936E+00	.7333E-01	.1027E+01	.1028E+01
.320	.1041E+00	.8704E-01	.3365E-01	.1031E+01	.1033E+01
.360	.1525E-01	.1275E-01	.5003E-02	.1034E+01	.1035E+01
.400	.3525E-03	.2947E-03	.1159E-03	.1035E+01	.1035E+01
.440	.5709E-05	.4772E-05	.1877E-05	.1035E+01	.1035E+01
.480	.9168E-07	.7665E-07	.3014E-07	.1035E+01	.1035E+01
.520	.1472E-08	.1231E-08	.4840E-09	.1035E+01	.1035E+01
.560	.2364E-10	.1977E-10	.7772E-11	.1035E+01	.1035E+01
.600	.3797E-12	.3174E-12	.1248E-12	.1035E+01	.1035E+01
.640	.6097E-14	.5097E-14	.2004E-14	.1035E+01	.1035E+01
.680	.9791E-16	.8185E-16	.3219E-16	.1035E+01	.1035E+01
.720	.1572E-17	.1314E-17	.5169E-18	.1035E+01	.1035E+01
.760	.2525E-19	.2111E-19	.8300E-20	.1035E+01	.1035E+01
.800	.4055E-21	.3390E-21	.1333E-21	.1035E+01	.1035E+01

.840	.6511E-23	.5443E-23	.2140E-23	.1035E+01	.1035E+01
.880	.1046E-24	.8742E-25	.3437E-25	.1035E+01	.1035E+01
.920	.1679E-26	.1404E-26	.5520E-27	.1035E+01	.1035E+01
.960	.2697E-28	.2254E-28	.8864E-29	.1035E+01	.1035E+01
1.000	.4330E-30	.3620E-30	.1423E-30	.1035E+01	.1035E+01

<< AT SULFIDATION TIME = 3.000 (hr) >>

(Z)	(CAB)	(X)	(SL)	(TG)	(TS)
.000	.1000E+01	.9567E+00	.3164E+00	.1000E+01	.1001E+01
.040	.9495E+00	.9084E+00	.3029E+00	.1002E+01	.1002E+01
.080	.8888E+00	.8503E+00	.2863E+00	.1004E+01	.1005E+01
.120	.8187E+00	.7832E+00	.2667E+00	.1006E+01	.1007E+01
.160	.7397E+00	.7076E+00	.2442E+00	.1009E+01	.1010E+01
.200	.6521E+00	.6238E+00	.2184E+00	.1012E+01	.1013E+01
.240	.5563E+00	.5322E+00	.1894E+00	.1015E+01	.1017E+01
.280	.4527E+00	.4331E+00	.1569E+00	.1019E+01	.1020E+01
.320	.3425E+00	.3276E+00	.1210E+00	.1023E+01	.1024E+01
.360	.2276E+00	.2177E+00	.8209E-01	.1027E+01	.1028E+01
.400	.1141E+00	.1091E+00	.4200E-01	.1031E+01	.1032E+01
.440	.2419E-01	.2315E-01	.9060E-02	.1034E+01	.1035E+01
.480	.7489E-03	.7161E-03	.2816E-03	.1035E+01	.1035E+01
.520	.1228E-04	.1174E-04	.4616E-05	.1035E+01	.1035E+01
.560	.1972E-06	.1886E-06	.7415E-07	.1035E+01	.1035E+01
.600	.3167E-08	.3028E-08	.1191E-08	.1035E+01	.1035E+01
.640	.5086E-10	.4863E-10	.1912E-10	.1035E+01	.1035E+01
.680	.8167E-12	.7809E-12	.3071E-12	.1035E+01	.1035E+01
.720	.1312E-13	.1254E-13	.4931E-14	.1035E+01	.1035E+01

.760	.2106E-15	.2014E-15	.7919E-16	.1035E+01	.1035E+01
.800	.3382E-17	.3234E-17	.1272E-17	.1035E+01	.1035E+01
.840	.5431E-19	.5193E-19	.2042E-19	.1035E+01	.1035E+01
.880	.8722E-21	.8340E-21	.3279E-21	.1035E+01	.1035E+01
.920	.1401E-22	.1339E-22	.5266E-23	.1035E+01	.1035E+01
.960	.2249E-24	.2151E-24	.8457E-25	.1035E+01	.1035E+01
1.000	.3612E-26	.3454E-26	.1358E-26	.1035E+01	.1035E+01

<< AT SULFIDATION TIME = 4.000 (hr) >>

(Z)	(CAB)	(X)	(SL)	(TG)	(TS)
.000	.1000E+01	.1000E+01	.3284E+00	.1000E+01	.1000E+01
.040	.9940E+00	.9937E+00	.3267E+00	.1000E+01	.1001E+01
.080	.9579E+00	.9576E+00	.3167E+00	.1002E+01	.1002E+01
.120	.9098E+00	.9095E+00	.3032E+00	.1003E+01	.1004E+01
.160	.8519E+00	.8517E+00	.2867E+00	.1005E+01	.1006E+01
.200	.7851E+00	.7848E+00	.2672E+00	.1008E+01	.1009E+01
.240	.7096E+00	.7094E+00	.2447E+00	.1010E+01	.1011E+01
.280	.6260E+00	.6258E+00	.2190E+00	.1013E+01	.1014E+01
.320	.5344E+00	.5343E+00	.1900E+00	.1016E+01	.1018E+01
.360	.4355E+00	.4354E+00	.1577E+00	.1020E+01	.1021E+01
.400	.3301E+00	.3300E+00	.1218E+00	.1024E+01	.1025E+01
.440	.2203E+00	.2202E+00	.8297E-01	.1028E+01	.1029E+01
.480	.1115E+00	.1114E+00	.4287E-01	.1031E+01	.1033E+01
.520	.2443E-01	.2442E-01	.9558E-02	.1034E+01	.1035E+01
.560	.7837E-03	.7831E-03	.3079E-03	.1035E+01	.1035E+01
.600	.1287E-04	.1286E-04	.5057E-05	.1035E+01	.1035E+01
.640	.2068E-06	.2066E-06	.8124E-07	.1035E+01	.1035E+01

.680	.3321E-08	.3318E-08	.1305E-08	.1035E+01	.1035E+01
.720	.5333E-10	.5328E-10	.2095E-10	.1035E+01	.1035E+01
.760	.8563E-12	.8556E-12	.3365E-12	.1035E+01	.1035E+01
.800	.1375E-13	.1374E-13	.5403E-14	.1035E+01	.1035E+01
.840	.2208E-15	.2207E-15	.8676E-16	.1035E+01	.1035E+01
.880	.3546E-17	.3543E-17	.1393E-17	.1035E+01	.1035E+01
.920	.5695E-19	.5690E-19	.2237E-19	.1035E+01	.1035E+01
.960	.9145E-21	.9138E-21	.3593E-21	.1035E+01	.1035E+01
1.000	.1469E-22	.1467E-22	.5770E-23	.1035E+01	.1035E+01

<< AT SULFIDATION TIME = 5.000 (hr) >>

(Z)	(CAB)	(X)	(SL)	(TG)	(TS)
.000	.1000E+01	.1000E+01	.3284E+00	.1000E+01	.1000E+01
.040	.1000E+01	.1000E+01	.3284E+00	.1000E+01	.1000E+01
.080	.1000E+01	.1000E+01	.3284E+00	.1000E+01	.1000E+01
.120	.9939E+00	.9936E+00	.3266E+00	.1000E+01	.1001E+01
.160	.9578E+00	.9575E+00	.3167E+00	.1002E+01	.1002E+01
.200	.9097E+00	.9094E+00	.3032E+00	.1003E+01	.1004E+01
.240	.8518E+00	.8515E+00	.2867E+00	.1005E+01	.1006E+01
.280	.7849E+00	.7846E+00	.2672E+00	.1008E+01	.1009E+01
.320	.7094E+00	.7092E+00	.2446E+00	.1010E+01	.1011E+01
.360	.6258E+00	.6255E+00	.2189E+00	.1013E+01	.1014E+01
.400	.5342E+00	.5340E+00	.1900E+00	.1016E+01	.1018E+01
.440	.4353E+00	.4351E+00	.1576E+00	.1020E+01	.1021E+01
.480	.3298E+00	.3297E+00	.1217E+00	.1024E+01	.1025E+01
.520	.2200E+00	.2199E+00	.8286E-01	.1028E+01	.1029E+01
.560	.1112E+00	.1111E+00	.4276E-01	.1031E+01	.1033E+01

.600	.2427E-01	.2426E-01	.9494E-02	.1034E+01	.1035E+01
.640	.7749E-03	.7743E-03	.3044E-03	.1035E+01	.1035E+01
.680	.1273E-04	.1271E-04	.4999E-05	.1035E+01	.1035E+01
.720	.2044E-06	.2042E-06	.8031E-07	.1035E+01	.1035E+01
.760	.3283E-08	.3280E-08	.1290E-08	.1035E+01	.1035E+01
.800	.5272E-10	.5267E-10	.2071E-10	.1035E+01	.1035E+01
.840	.8466E-12	.8458E-12	.3326E-12	.1035E+01	.1035E+01
.880	.1359E-13	.1358E-13	.5341E-14	.1035E+01	.1035E+01
.920	.2183E-15	.2181E-15	.8577E-16	.1035E+01	.1035E+01
.960	.3506E-17	.3503E-17	.1377E-17	.1035E+01	.1035E+01
1.000	.5630E-19	.5625E-19	.2212E-19	.1035E+01	.1035E+01

<< AT SULFIDATION TIME = 6.000 (hr) >>

(Z)	(CAB)	(X)	(SL)	(TG)	(TS)
.000	.1000E+01	.1000E+01	.3284E+00	.1000E+01	.1000E+01
.040	.1000E+01	.1000E+01	.3284E+00	.1000E+01	.1000E+01
.080	.1000E+01	.1000E+01	.3284E+00	.1000E+01	.1000E+01
.120	.1000E+01	.1000E+01	.3284E+00	.1000E+01	.1000E+01
.160	.1000E+01	.1000E+01	.3284E+00	.1000E+01	.1000E+01
.200	.9939E+00	.9935E+00	.3266E+00	.1000E+01	.1001E+01
.240	.9578E+00	.9574E+00	.3166E+00	.1002E+01	.1002E+01
.280	.9096E+00	.9092E+00	.3031E+00	.1003E+01	.1004E+01
.320	.8517E+00	.8513E+00	.2866E+00	.1005E+01	.1006E+01
.360	.7847E+00	.7844E+00	.2671E+00	.1008E+01	.1009E+01
.400	.7093E+00	.7090E+00	.2446E+00	.1010E+01	.1011E+01
.440	.6256E+00	.6253E+00	.2189E+00	.1013E+01	.1014E+01
.480	.5340E+00	.5337E+00	.1899E+00	.1016E+01	.1018E+01

.520	.4350E+00	.4348E+00	.1575E+00	.1020E+01	.1021E+01
.560	.3295E+00	.3294E+00	.1216E+00	.1024E+01	.1025E+01
.600	.2197E+00	.2196E+00	.8275E-01	.1028E+01	.1029E+01
.640	.1109E+00	.1108E+00	.4265E-01	.1031E+01	.1033E+01
.680	.2411E-01	.2410E-01	.9430E-02	.1034E+01	.1035E+01
.720	.7662E-03	.7656E-03	.3010E-03	.1035E+01	.1035E+01
.760	.1258E-04	.1257E-04	.4942E-05	.1035E+01	.1035E+01
.800	.2021E-06	.2019E-06	.7939E-07	.1035E+01	.1035E+01
.840	.3245E-08	.3242E-08	.1275E-08	.1035E+01	.1035E+01
.880	.5211E-10	.5206E-10	.2047E-10	.1035E+01	.1035E+01
.920	.8369E-12	.8361E-12	.3288E-12	.1035E+01	.1035E+01
.960	.1344E-13	.1343E-13	.5279E-14	.1035E+01	.1035E+01
1.000	.2158E-15	.2156E-15	.8478E-16	.1035E+01	.1035E+01

<< AT SULFIDATION TIME = 7.000 (hr) >>

(Z)	(CAB)	(X)	(SL)	(TG)	(TS)
.000	.1000E+01	.1000E+01	.3284E+00	.1000E+01	.1000E+01
.040	.1000E+01	.1000E+01	.3284E+00	.1000E+01	.1000E+01
.080	.1000E+01	.1000E+01	.3284E+00	.1000E+01	.1000E+01
.120	.1000E+01	.1000E+01	.3284E+00	.1000E+01	.1000E+01
.160	.1000E+01	.1000E+01	.3284E+00	.1000E+01	.1000E+01
.200	.1000E+01	.1000E+01	.3284E+00	.1000E+01	.1000E+01
.240	.1000E+01	.1000E+01	.3284E+00	.1000E+01	.1000E+01
.280	.9939E+00	.9934E+00	.3266E+00	.1000E+01	.1001E+01
.320	.9577E+00	.9572E+00	.3166E+00	.1002E+01	.1002E+01
.360	.9095E+00	.9091E+00	.3031E+00	.1003E+01	.1004E+01
.400	.8515E+00	.8511E+00	.2865E+00	.1005E+01	.1006E+01

.440	.7846E+00	.7842E+00	.2670E+00	.1008E+01	.1009E+01
.480	.7091E+00	.7087E+00	.2445E+00	.1010E+01	.1011E+01
.520	.6253E+00	.6250E+00	.2188E+00	.1013E+01	.1014E+01
.560	.5337E+00	.5335E+00	.1898E+00	.1016E+01	.1018E+01
.600	.4347E+00	.4345E+00	.1574E+00	.1020E+01	.1021E+01
.640	.3293E+00	.3291E+00	.1215E+00	.1024E+01	.1025E+01
.680	.2194E+00	.2193E+00	.8264E-01	.1028E+01	.1029E+01
.720	.1106E+00	.1105E+00	.4254E-01	.1031E+01	.1033E+01
.760	.2394E-01	.2393E-01	.9367E-02	.1034E+01	.1035E+01
.800	.7576E-03	.7570E-03	.2976E-03	.1035E+01	.1035E+01
.840	.1244E-04	.1242E-04	.4885E-05	.1035E+01	.1035E+01
.880	.1998E-06	.1996E-06	.7847E-07	.1035E+01	.1035E+01
.920	.3208E-08	.3205E-08	.1260E-08	.1035E+01	.1035E+01
.960	.5152E-10	.5146E-10	.2024E-10	.1035E+01	.1035E+01
1.000	.8273E-12	.8265E-12	.3250E-12	.1035E+01	.1035E+01

<< AT SULFIDATION TIME = 8.000 (hr) >>

(Z)	(CAB)	(X)	(SL)	(TG)	(TS)
.000	.1000E+01	.1000E+01	.3284E+00	.1000E+01	.1000E+01
.040	.1000E+01	.1000E+01	.3284E+00	.1000E+01	.1000E+01
.080	.1000E+01	.1000E+01	.3284E+00	.1000E+01	.1000E+01
.120	.1000E+01	.1000E+01	.3284E+00	.1000E+01	.1000E+01
.160	.1000E+01	.1000E+01	.3284E+00	.1000E+01	.1000E+01
.200	.1000E+01	.1000E+01	.3284E+00	.1000E+01	.1000E+01
.240	.1000E+01	.1000E+01	.3284E+00	.1000E+01	.1000E+01
.280	.1000E+01	.1000E+01	.3284E+00	.1000E+01	.1000E+01
.320	.1000E+01	.1000E+01	.3284E+00	.1000E+01	.1000E+01

.360	.9939E+00	.9933E+00	.3266E+00	.1000E+01	.1001E+01
.400	.9576E+00	.9571E+00	.3166E+00	.1002E+01	.1002E+01
.440	.9094E+00	.9089E+00	.3030E+00	.1003E+01	.1004E+01
.480	.8514E+00	.8510E+00	.2865E+00	.1005E+01	.1006E+01
.520	.7844E+00	.7840E+00	.2670E+00	.1008E+01	.1009E+01
.560	.7089E+00	.7085E+00	.2444E+00	.1010E+01	.1011E+01
.600	.6251E+00	.6248E+00	.2187E+00	.1013E+01	.1014E+01
.640	.5335E+00	.5332E+00	.1897E+00	.1017E+01	.1018E+01
.680	.4345E+00	.4342E+00	.1573E+00	.1020E+01	.1021E+01
.720	.3290E+00	.3288E+00	.1214E+00	.1024E+01	.1025E+01
.760	.2191E+00	.2189E+00	.8253E-01	.1028E+01	.1029E+01
.800	.1103E+00	.1103E+00	.4243E-01	.1031E+01	.1033E+01
.840	.2378E-01	.2377E-01	.9304E-02	.1034E+01	.1035E+01
.880	.7491E-03	.7485E-03	.2943E-03	.1035E+01	.1035E+01
.920	.1229E-04	.1228E-04	.4829E-05	.1035E+01	.1035E+01
.960	.1975E-06	.1973E-06	.7757E-07	.1035E+01	.1035E+01
1.000	.3171E-08	.3168E-08	.1246E-08	.1035E+01	.1035E+01

<< AT SULFIDATION TIME = 9.000 (hr) >>

(Z)	(CAB)	(X)	(SL)	(TG)	(TS)
.000	.1000E+01	.1000E+01	.3284E+00	.1000E+01	.1000E+01
.040	.1000E+01	.1000E+01	.3284E+00	.1000E+01	.1000E+01
.080	.1000E+01	.1000E+01	.3284E+00	.1000E+01	.1000E+01
.120	.1000E+01	.1000E+01	.3284E+00	.1000E+01	.1000E+01
.160	.1000E+01	.1000E+01	.3284E+00	.1000E+01	.1000E+01
.200	.1000E+01	.1000E+01	.3284E+00	.1000E+01	.1000E+01
.240	.1000E+01	.1000E+01	.3284E+00	.1000E+01	.1000E+01

.280	.1000E+01	.1000E+01	.3284E+00	.1000E+01	.1000E+01
.320	.1000E+01	.1000E+01	.3284E+00	.1000E+01	.1000E+01
.360	.1000E+01	.1000E+01	.3284E+00	.1000E+01	.1000E+01
.400	.1000E+01	.1000E+01	.3284E+00	.1000E+01	.1000E+01
.440	.9938E+00	.9933E+00	.3266E+00	.1000E+01	.1001E+01
.480	.9576E+00	.9570E+00	.3165E+00	.1002E+01	.1002E+01
.520	.9093E+00	.9088E+00	.3030E+00	.1003E+01	.1004E+01
.560	.8513E+00	.8508E+00	.2864E+00	.1005E+01	.1006E+01
.600	.7843E+00	.7838E+00	.2669E+00	.1008E+01	.1009E+01
.640	.7087E+00	.7083E+00	.2444E+00	.1010E+01	.1011E+01
.680	.6249E+00	.6246E+00	.2186E+00	.1013E+01	.1015E+01
.720	.5333E+00	.5329E+00	.1896E+00	.1017E+01	.1018E+01
.760	.4342E+00	.4339E+00	.1572E+00	.1020E+01	.1021E+01
.800	.3287E+00	.3285E+00	.1213E+00	.1024E+01	.1025E+01
.840	.2188E+00	.2186E+00	.8241E-01	.1028E+01	.1029E+01
.880	.1100E+00	.1100E+00	.4232E-01	.1031E+01	.1033E+01
.920	.2362E-01	.2361E-01	.9241E-02	.1034E+01	.1035E+01
.960	.7407E-03	.7400E-03	.2910E-03	.1035E+01	.1035E+01
1.000	.1215E-04	.1214E-04	.4773E-05	.1035E+01	.1035E+01

<< AT SULFIDATION TIME = 10.000 (hr) >>

(Z)	(CAB)	(X)	(SL)	(TG)	(TS)
.000	.1000E+01	.1000E+01	.3284E+00	.1000E+01	.1000E+01
.040	.1000E+01	.1000E+01	.3284E+00	.1000E+01	.1000E+01
.080	.1000E+01	.1000E+01	.3284E+00	.1000E+01	.1000E+01
.120	.1000E+01	.1000E+01	.3284E+00	.1000E+01	.1000E+01
.160	.1000E+01	.1000E+01	.3284E+00	.1000E+01	.1000E+01

.200	.1000E+01	.1000E+01	.3284E+00	.1000E+01	.1000E+01
.240	.1000E+01	.1000E+01	.3284E+00	.1000E+01	.1000E+01
.280	.1000E+01	.1000E+01	.3284E+00	.1000E+01	.1000E+01
.320	.1000E+01	.1000E+01	.3284E+00	.1000E+01	.1000E+01
.360	.1000E+01	.1000E+01	.3284E+00	.1000E+01	.1000E+01
.400	.1000E+01	.1000E+01	.3284E+00	.1000E+01	.1000E+01
.440	.1000E+01	.1000E+01	.3284E+00	.1000E+01	.1000E+01
.480	.1000E+01	.1000E+01	.3284E+00	.1000E+01	.1000E+01
.520	.9938E+00	.9932E+00	.3265E+00	.1000E+01	.1001E+01
.560	.9575E+00	.9569E+00	.3165E+00	.1002E+01	.1002E+01
.600	.9092E+00	.9086E+00	.3030E+00	.1003E+01	.1004E+01
.640	.8512E+00	.8506E+00	.2864E+00	.1005E+01	.1006E+01
.680	.7841E+00	.7836E+00	.2669E+00	.1008E+01	.1009E+01
.720	.7085E+00	.7081E+00	.2443E+00	.1010E+01	.1011E+01
.760	.6247E+00	.6243E+00	.2186E+00	.1013E+01	.1015E+01
.800	.5330E+00	.5327E+00	.1895E+00	.1017E+01	.1018E+01
.840	.4339E+00	.4337E+00	.1571E+00	.1020E+01	.1021E+01
.880	.3284E+00	.3282E+00	.1212E+00	.1024E+01	.1025E+01
.920	.2185E+00	.2183E+00	.8230E-01	.1028E+01	.1029E+01
.960	.1097E+00	.1097E+00	.4221E-01	.1031E+01	.1033E+01
1.000	.2346E-01	.2345E-01	.9178E-02	.1034E+01	.1035E+01

Section 5

<< AT BED LOCATION = .100 >>

TIME (HR)	GAS TEMP (TG)	SORBENT TEMP (TS)
.4000	.1023E+01	.1027E+01
.8000	.1015E+01	.1018E+01
1.2000	.1012E+01	.1014E+01
1.6000	.1009E+01	.1011E+01
2.0000	.1008E+01	.1009E+01
2.4000	.1006E+01	.1008E+01
2.8000	.1005E+01	.1006E+01
3.2000	.1004E+01	.1005E+01
3.6000	.1004E+01	.1004E+01
4.0000	.1002E+01	.1003E+01
4.4000	.1001E+01	.1002E+01
4.8000	.1000E+01	.1001E+01
5.2000	.1000E+01	.1000E+01
5.6000	.1000E+01	.1000E+01
6.0000	.1000E+01	.1000E+01
6.4000	.1000E+01	.1000E+01
6.8000	.1000E+01	.1000E+01
7.2000	.1000E+01	.1000E+01
7.6000	.1000E+01	.1000E+01
8.0000	.1000E+01	.1000E+01
8.4000	.1000E+01	.1000E+01
8.8000	.1000E+01	.1000E+01
9.2000	.1000E+01	.1000E+01
9.6000	.1000E+01	.1000E+01
10.0000	.1000E+01	.1000E+01
10.4000	.1000E+01	.1000E+01
10.8000	.1000E+01	.1000E+01
11.2000	.1000E+01	.1000E+01
11.6000	.1000E+01	.1000E+01
12.0000	.1000E+01	.1000E+01
12.4000	.1000E+01	.1000E+01
12.8000	.1000E+01	.1000E+01
13.2000	.1000E+01	.1000E+01
13.6000	.1000E+01	.1000E+01
14.0000	.1000E+01	.1000E+01
14.4000	.1000E+01	.1000E+01
14.8000	.1000E+01	.1000E+01
15.2000	.1000E+01	.1000E+01
15.6000	.1000E+01	.1000E+01
16.0000	.1000E+01	.1000E+01
16.4000	.1000E+01	.1000E+01
16.8000	.1000E+01	.1000E+01
17.2000	.1000E+01	.1000E+01
17.6000	.1000E+01	.1000E+01

18.0000	.1000E+01	.1000E+01
18.4000	.1000E+01	.1000E+01
18.8000	.1000E+01	.1000E+01
19.2000	.1000E+01	.1000E+01
19.6000	.1000E+01	.1000E+01
20.0000	.1000E+01	.1000E+01

<< AT BED LOCATION = 200 >>

TIME (HR)	GAS TEMP (TG)	SORBENT TEMP (TS)
.4000	.1036E+01	.1036E+01
.8000	.1032E+01	.1034E+01
1.2000	.1025E+01	.1028E+01
1.6000	.1021E+01	.1023E+01
2.0000	.1017E+01	.1019E+01
2.4000	.1015E+01	.1016E+01
2.8000	.1013E+01	.1014E+01
3.2000	.1011E+01	.1012E+01
3.6000	.1009E+01	.1011E+01
4.0000	.1008E+01	.1009E+01
4.4000	.1006E+01	.1007E+01
4.8000	.1004E+01	.1005E+01
5.2000	.1003E+01	.1003E+01
5.6000	.1001E+01	.1002E+01
6.0000	.1000E+01	.1001E+01
6.4000	.1000E+01	.1000E+01
6.8000	.1000E+01	.1000E+01
7.2000	.1000E+01	.1000E+01
7.6000	.1000E+01	.1000E+01
8.0000	.1000E+01	.1000E+01
8.4000	.1000E+01	.1000E+01
8.8000	.1000E+01	.1000E+01
9.2000	.1000E+01	.1000E+01
9.6000	.1000E+01	.1000E+01
10.0000	.1000E+01	.1000E+01
10.4000	.1000E+01	.1000E+01
10.8000	.1000E+01	.1000E+01
11.2000	.1000E+01	.1000E+01
11.6000	.1000E+01	.1000E+01
12.0000	.1000E+01	.1000E+01
12.4000	.1000E+01	.1000E+01
12.8000	.1000E+01	.1000E+01
13.2000	.1000E+01	.1000E+01
13.6000	.1000E+01	.1000E+01
14.0000	.1000E+01	.1000E+01
14.4000	.1000E+01	.1000E+01
14.8000	.1000E+01	.1000E+01
15.2000	.1000E+01	.1000E+01
15.6000	.1000E+01	.1000E+01
16.0000	.1000E+01	.1000E+01
16.4000	.1000E+01	.1000E+01

16.8000	.1000E+01	.1000E+01
17.2000	.1000E+01	.1000E+01
17.6000	.1000E+01	.1000E+01
18.0000	.1000E+01	.1000E+01
18.4000	.1000E+01	.1000E+01
18.8000	.1000E+01	.1000E+01
19.2000	.1000E+01	.1000E+01
19.6000	.1000E+01	.1000E+01
20.0000	.1000E+01	.1000E+01

<< AT BED LOCATION = .300 >>

TIME (HR)	GAS TEMP (TG)	SORBENT TEMP (TS)
.4000	.1036E+01	.1036E+01
.8000	.1035E+01	.1035E+01
1.2000	.1035E+01	.1035E+01
1.6000	.1033E+01	.1034E+01
2.0000	.1029E+01	.1031E+01
2.4000	.1025E+01	.1027E+01
2.8000	.1022E+01	.1024E+01
3.2000	.1019E+01	.1021E+01
3.6000	.1017E+01	.1018E+01
4.0000	.1015E+01	.1016E+01
4.4000	.1012E+01	.1014E+01
4.8000	.1010E+01	.1011E+01
5.2000	.1008E+01	.1009E+01
5.6000	.1006E+01	.1007E+01
6.0000	.1004E+01	.1005E+01
6.4000	.1003E+01	.1003E+01
6.8000	.1001E+01	.1002E+01
7.2000	.1000E+01	.1001E+01
7.6000	.1000E+01	.1000E+01
8.0000	.1000E+01	.1000E+01
8.4000	.1000E+01	.1000E+01
8.8000	.1000E+01	.1000E+01
9.2000	.1000E+01	.1000E+01
9.6000	.1000E+01	.1000E+01
10.0000	.1000E+01	.1000E+01
10.4000	.1000E+01	.1000E+01
10.8000	.1000E+01	.1000E+01
11.2000	.1000E+01	.1000E+01
11.6000	.1000E+01	.1000E+01
12.0000	.1000E+01	.1000E+01
12.4000	.1000E+01	.1000E+01
12.8000	.1000E+01	.1000E+01
13.2000	.1000E+01	.1000E+01
13.6000	.1000E+01	.1000E+01
14.0000	.1000E+01	.1000E+01
14.4000	.1000E+01	.1000E+01
14.8000	.1000E+01	.1000E+01
15.2000	.1000E+01	.1000E+01

15.6000	.1000E+01	.1000E+01
16.0000	.1000E+01	.1000E+01
16.4000	.1000E+01	.1000E+01
16.8000	.1000E+01	.1000E+01
17.2000	.1000E+01	.1000E+01
17.6000	.1000E+01	.1000E+01
18.0000	.1000E+01	.1000E+01
18.4000	.1000E+01	.1000E+01
18.8000	.1000E+01	.1000E+01
19.2000	.1000E+01	.1000E+01
19.6000	.1000E+01	.1000E+01
20.0000	.1000E+01	.1000E+01

<< AT BED LOCATION = .400 >>

TIME (HR)	GAS TEMP (TG)	SORBENT TEMP (TS)
.4000	.1036E+01	.1035E+01
.8000	.1035E+01	.1035E+01
1.2000	.1035E+01	.1035E+01
1.6000	.1035E+01	.1035E+01
2.0000	.1035E+01	.1035E+01
2.4000	.1034E+01	.1035E+01
2.8000	.1032E+01	.1034E+01
3.2000	.1029E+01	.1031E+01
3.6000	.1026E+01	.1028E+01
4.0000	.1024E+01	.1025E+01
4.4000	.1021E+01	.1022E+01
4.8000	.1018E+01	.1019E+01
5.2000	.1015E+01	.1016E+01
5.6000	.1013E+01	.1014E+01
6.0000	.1010E+01	.1011E+01
6.4000	.1008E+01	.1009E+01
6.8000	.1006E+01	.1007E+01
7.2000	.1004E+01	.1005E+01
7.6000	.1003E+01	.1004E+01
8.0000	.1002E+01	.1002E+01
8.4000	.1000E+01	.1001E+01
8.8000	.1000E+01	.1000E+01
9.2000	.1000E+01	.1000E+01
9.6000	.1000E+01	.1000E+01
10.0000	.1000E+01	.1000E+01
10.4000	.1000E+01	.1000E+01
10.8000	.1000E+01	.1000E+01
11.2000	.1000E+01	.1000E+01
11.6000	.1000E+01	.1000E+01
12.0000	.1000E+01	.1000E+01
12.4000	.1000E+01	.1000E+01
12.8000	.1000E+01	.1000E+01
13.2000	.1000E+01	.1000E+01
13.6000	.1000E+01	.1000E+01
14.0000	.1000E+01	.1000E+01

14.4000	.1000E+01	.1000E+01
14.8000	.1000E+01	.1000E+01
15.2000	.1000E+01	.1000E+01
15.6000	.1000E+01	.1000E+01
16.0000	.1000E+01	.1000E+01
16.4000	.1000E+01	.1000E+01
16.8000	.1000E+01	.1000E+01
17.2000	.1000E+01	.1000E+01
17.6000	.1000E+01	.1000E+01
18.0000	.1000E+01	.1000E+01
18.4000	.1000E+01	.1000E+01
18.8000	.1000E+01	.1000E+01
19.2000	.1000E+01	.1000E+01
19.6000	.1000E+01	.1000E+01
20.0000	.1000E+01	.1000E+01

<< AT BED LOCATION = .500 >>

TIME (HR)	GAS TEMP (TG)	SORBENT TEMP (TS)
.4000	.1030E+01	.1029E+01
.8000	.1035E+01	.1036E+01
1.2000	.1035E+01	.1035E+01
1.6000	.1035E+01	.1035E+01
2.0000	.1035E+01	.1035E+01
2.4000	.1035E+01	.1035E+01
2.8000	.1035E+01	.1035E+01
3.2000	.1035E+01	.1035E+01
3.6000	.1034E+01	.1035E+01
4.0000	.1033E+01	.1034E+01
4.4000	.1030E+01	.1032E+01
4.8000	.1027E+01	.1029E+01
5.2000	.1024E+01	.1026E+01
5.6000	.1021E+01	.1022E+01
6.0000	.1018E+01	.1020E+01
6.4000	.1015E+01	.1017E+01
6.8000	.1013E+01	.1014E+01
7.2000	.1011E+01	.1012E+01
7.6000	.1008E+01	.1009E+01
8.0000	.1006E+01	.1007E+01
8.4000	.1005E+01	.1005E+01
8.8000	.1003E+01	.1004E+01
9.2000	.1002E+01	.1002E+01
9.6000	.1001E+01	.1001E+01
10.0000	.1000E+01	.1000E+01
10.4000	.1000E+01	.1000E+01
10.8000	.1000E+01	.1000E+01
11.2000	.1000E+01	.1000E+01
11.6000	.1000E+01	.1000E+01
12.0000	.1000E+01	.1000E+01
12.4000	.1000E+01	.1000E+01
12.8000	.1000E+01	.1000E+01

13.2000	.1000E+01	.1000E+01
13.6000	.1000E+01	.1000E+01
14.0000	.1000E+01	.1000E+01
14.4000	.1000E+01	.1000E+01
14.8000	.1000E+01	.1000E+01
15.2000	.1000E+01	.1000E+01
15.6000	.1000E+01	.1000E+01
16.0000	.1000E+01	.1000E+01
16.4000	.1000E+01	.1000E+01
16.8000	.1000E+01	.1000E+01
17.2000	.1000E+01	.1000E+01
17.6000	.1000E+01	.1000E+01
18.0000	.1000E+01	.1000E+01
18.4000	.1000E+01	.1000E+01
18.8000	.1000E+01	.1000E+01
19.2000	.1000E+01	.1000E+01
19.6000	.1000E+01	.1000E+01
20.0000	.1000E+01	.1000E+01

<< AT BED LOCATION = .600 >>

TIME (HR)	GAS TEMP (TG)	SORBENT TEMP (TS)
.4000	.1020E+01	.1018E+01
.8000	.1036E+01	.1036E+01
1.2000	.1035E+01	.1035E+01
1.6000	.1035E+01	.1035E+01
2.0000	.1035E+01	.1035E+01
2.4000	.1035E+01	.1035E+01
2.8000	.1035E+01	.1035E+01
3.2000	.1035E+01	.1035E+01
3.6000	.1035E+01	.1035E+01
4.0000	.1035E+01	.1035E+01
4.4000	.1035E+01	.1035E+01
4.8000	.1035E+01	.1035E+01
5.2000	.1033E+01	.1035E+01
5.6000	.1031E+01	.1032E+01
6.0000	.1028E+01	.1029E+01
6.4000	.1024E+01	.1026E+01
6.8000	.1021E+01	.1023E+01
7.2000	.1019E+01	.1020E+01
7.6000	.1016E+01	.1017E+01
8.0000	.1013E+01	.1014E+01
8.4000	.1011E+01	.1012E+01
8.8000	.1009E+01	.1010E+01
9.2000	.1007E+01	.1008E+01
9.6000	.1005E+01	.1006E+01
10.0000	.1003E+01	.1004E+01
10.4000	.1002E+01	.1003E+01
10.8000	.1001E+01	.1001E+01
11.2000	.1000E+01	.1000E+01
11.6000	.1000E+01	.1000E+01

12.0000	.1000E+01	.1000E+01
12.4000	.1000E+01	.1000E+01
12.8000	.1000E+01	.1000E+01
13.2000	.1000E+01	.1000E+01
13.6000	.1000E+01	.1000E+01
14.0000	.1000E+01	.1000E+01
14.4000	.1000E+01	.1000E+01
14.8000	.1000E+01	.1000E+01
15.2000	.1000E+01	.1000E+01
15.6000	.1000E+01	.1000E+01
16.0000	.1000E+01	.1000E+01
16.4000	.1000E+01	.1000E+01
16.8000	.1000E+01	.1000E+01
17.2000	.1000E+01	.1000E+01
17.6000	.1000E+01	.1000E+01
18.0000	.1000E+01	.1000E+01
18.4000	.1000E+01	.1000E+01
18.8000	.1000E+01	.1000E+01
19.2000	.1000E+01	.1000E+01
19.6000	.1000E+01	.1000E+01
20.0000	.1000E+01	.1000E+01

<< AT BED LOCATION = .700 >>

TIME (HR)	GAS TEMP (TG)	SORBENT TEMP (TS)
.4000	.1009E+01	.1008E+01
.8000	.1036E+01	.1036E+01
1.2000	.1035E+01	.1035E+01
1.6000	.1035E+01	.1035E+01
2.0000	.1035E+01	.1035E+01
2.4000	.1035E+01	.1035E+01
2.8000	.1035E+01	.1035E+01
3.2000	.1035E+01	.1035E+01
3.6000	.1035E+01	.1035E+01
4.0000	.1035E+01	.1035E+01
4.4000	.1035E+01	.1035E+01
4.8000	.1035E+01	.1035E+01
5.2000	.1035E+01	.1035E+01
5.6000	.1035E+01	.1035E+01
6.0000	.1035E+01	.1035E+01
6.4000	.1034E+01	.1035E+01
6.8000	.1031E+01	.1032E+01
7.2000	.1028E+01	.1029E+01
7.6000	.1025E+01	.1026E+01
8.0000	.1022E+01	.1023E+01
8.4000	.1019E+01	.1020E+01
8.8000	.1016E+01	.1017E+01
9.2000	.1014E+01	.1015E+01
9.6000	.1011E+01	.1012E+01
10.0000	.1009E+01	.1010E+01
10.4000	.1007E+01	.1008E+01

10.8000	.1005E+01	.1006E+01
11.2000	.1003E+01	.1004E+01
11.6000	.1002E+01	.1003E+01
12.0000	.1001E+01	.1001E+01
12.4000	.1000E+01	.1000E+01
12.8000	.1000E+01	.1000E+01
13.2000	.1000E+01	.1000E+01
13.6000	.1000E+01	.1000E+01
14.0000	.1000E+01	.1000E+01
14.4000	.1000E+01	.1000E+01
14.8000	.1000E+01	.1000E+01
15.2000	.1000E+01	.1000E+01
15.6000	.1000E+01	.1000E+01
16.0000	.1000E+01	.1000E+01
16.4000	.1000E+01	.1000E+01
16.8000	.1000E+01	.1000E+01
17.2000	.1000E+01	.1000E+01
17.6000	.1000E+01	.1000E+01
18.0000	.1000E+01	.1000E+01
18.4000	.1000E+01	.1000E+01
18.8000	.1000E+01	.1000E+01
19.2000	.1000E+01	.1000E+01
19.6000	.1000E+01	.1000E+01
20.0000	.1000E+01	.1000E+01

<< AT BED LOCATION = .800 >>

TIME (HR)	GAS TEMP (TG)	SORBENT TEMP (TS)
.4000	.1003E+01	.1003E+01
.8000	.1036E+01	.1036E+01
1.2000	.1035E+01	.1035E+01
1.6000	.1035E+01	.1035E+01
2.0000	.1035E+01	.1035E+01
2.4000	.1035E+01	.1035E+01
2.8000	.1035E+01	.1035E+01
3.2000	.1035E+01	.1035E+01
3.6000	.1035E+01	.1035E+01
4.0000	.1035E+01	.1035E+01
4.4000	.1035E+01	.1035E+01
4.8000	.1035E+01	.1035E+01
5.2000	.1035E+01	.1035E+01
5.6000	.1035E+01	.1035E+01
6.0000	.1035E+01	.1035E+01
6.4000	.1035E+01	.1035E+01
6.8000	.1035E+01	.1035E+01
7.2000	.1035E+01	.1035E+01
7.6000	.1034E+01	.1035E+01
8.0000	.1031E+01	.1033E+01
8.4000	.1028E+01	.1030E+01
8.8000	.1025E+01	.1027E+01
9.2000	.1022E+01	.1024E+01

9.6000	.1019E+01	.1021E+01
10.0000	.1017E+01	.1018E+01
10.4000	.1014E+01	.1015E+01
10.8000	.1012E+01	.1013E+01
11.2000	.1009E+01	.1010E+01
11.6000	.1007E+01	.1008E+01
12.0000	.1005E+01	.1006E+01
12.4000	.1004E+01	.1004E+01
12.8000	.1002E+01	.1003E+01
13.2000	.1001E+01	.1002E+01
13.6000	.1000E+01	.1000E+01
14.0000	.1000E+01	.1000E+01
14.4000	.1000E+01	.1000E+01
14.8000	.1000E+01	.1000E+01
15.2000	.1000E+01	.1000E+01
15.6000	.1000E+01	.1000E+01
16.0000	.1000E+01	.1000E+01
16.4000	.1000E+01	.1000E+01
16.8000	.1000E+01	.1000E+01
17.2000	.1000E+01	.1000E+01
17.6000	.1000E+01	.1000E+01
18.0000	.1000E+01	.1000E+01
18.4000	.1000E+01	.1000E+01
18.8000	.1000E+01	.1000E+01
19.2000	.1000E+01	.1000E+01
19.6000	.1000E+01	.1000E+01
20.0000	.1000E+01	.1000E+01

<< AT BED LOCATION = .900 >>

TIME (HR)	GAS TEMP (TG)	SORBENT TEMP (TS)
.4000	.1001E+01	.1001E+01
.8000	.1035E+01	.1035E+01
1.2000	.1035E+01	.1035E+01
1.6000	.1035E+01	.1035E+01
2.0000	.1035E+01	.1035E+01
2.4000	.1035E+01	.1035E+01
2.8000	.1035E+01	.1035E+01
3.2000	.1035E+01	.1035E+01
3.6000	.1035E+01	.1035E+01
4.0000	.1035E+01	.1035E+01
4.4000	.1035E+01	.1035E+01
4.8000	.1035E+01	.1035E+01
5.2000	.1035E+01	.1035E+01
5.6000	.1035E+01	.1035E+01
6.0000	.1035E+01	.1035E+01
6.4000	.1035E+01	.1035E+01
6.8000	.1035E+01	.1035E+01
7.2000	.1035E+01	.1035E+01
7.6000	.1035E+01	.1035E+01
8.0000	.1035E+01	.1035E+01

8.4000	.1035E+01	.1035E+01
8.8000	.1034E+01	.1035E+01
9.2000	.1032E+01	.1033E+01
9.6000	.1029E+01	.1030E+01
10.0000	.1026E+01	.1027E+01
10.4000	.1023E+01	.1024E+01
10.8000	.1020E+01	.1021E+01
11.2000	.1017E+01	.1018E+01
11.6000	.1014E+01	.1016E+01
12.0000	.1012E+01	.1013E+01
12.4000	.1010E+01	.1011E+01
12.8000	.1007E+01	.1008E+01
13.2000	.1006E+01	.1006E+01
13.6000	.1004E+01	.1005E+01
14.0000	.1002E+01	.1003E+01
14.4000	.1001E+01	.1002E+01
14.8000	.1000E+01	.1001E+01
15.2000	.1000E+01	.1000E+01
15.6000	.1000E+01	.1000E+01
16.0000	.1000E+01	.1000E+01
16.4000	.1000E+01	.1000E+01
16.8000	.1000E+01	.1000E+01
17.2000	.1000E+01	.1000E+01
17.6000	.1000E+01	.1000E+01
18.0000	.1000E+01	.1000E+01
18.4000	.1000E+01	.1000E+01
18.8000	.1000E+01	.1000E+01
19.2000	.1000E+01	.1000E+01
19.6000	.1000E+01	.1000E+01
20.0000	.1000E+01	.1000E+01

<< AT BED LOCATION = 1.000 >>

TIME (HR)	GAS TEMP (TG)	SORBENT TEMP (TS)
.4000	.1000E+01	.1000E+01
.8000	.1032E+01	.1031E+01
1.2000	.1035E+01	.1035E+01
1.6000	.1035E+01	.1035E+01
2.0000	.1035E+01	.1035E+01
2.4000	.1035E+01	.1035E+01
2.8000	.1035E+01	.1035E+01
3.2000	.1035E+01	.1035E+01
3.6000	.1035E+01	.1035E+01
4.0000	.1035E+01	.1035E+01
4.4000	.1035E+01	.1035E+01
4.8000	.1035E+01	.1035E+01
5.2000	.1035E+01	.1035E+01
5.6000	.1035E+01	.1035E+01
6.0000	.1035E+01	.1035E+01
6.4000	.1035E+01	.1035E+01
6.8000	.1035E+01	.1035E+01

7.2000	.1035E+01	.1035E+01
7.6000	.1035E+01	.1035E+01
8.0000	.1035E+01	.1035E+01
8.4000	.1035E+01	.1035E+01
8.8000	.1035E+01	.1035E+01
9.2000	.1035E+01	.1035E+01
9.6000	.1035E+01	.1035E+01
10.0000	.1034E+01	.1035E+01
10.4000	.1032E+01	.1033E+01
10.8000	.1029E+01	.1031E+01
11.2000	.1026E+01	.1028E+01
11.6000	.1023E+01	.1024E+01
12.0000	.1020E+01	.1021E+01
12.4000	.1017E+01	.1019E+01
12.8000	.1015E+01	.1016E+01
13.2000	.1012E+01	.1013E+01
13.6000	.1010E+01	.1011E+01
14.0000	.1008E+01	.1009E+01
14.4000	.1006E+01	.1007E+01
14.8000	.1004E+01	.1005E+01
15.2000	.1003E+01	.1003E+01
15.6000	.1001E+01	.1002E+01
16.0000	.1000E+01	.1001E+01
16.4000	.1000E+01	.1000E+01
16.8000	.1000E+01	.1000E+01
17.2000	.1000E+01	.1000E+01
17.6000	.1000E+01	.1000E+01
18.0000	.1000E+01	.1000E+01
18.4000	.1000E+01	.1000E+01
18.8000	.1000E+01	.1000E+01
19.2000	.1000E+01	.1000E+01
19.6000	.1000E+01	.1000E+01
20.0000	.1000E+01	.1000E+01

APPENDIX D

PROGRAM FOR REGENERATION MODEL

C ***** ABSTRACT *****

C This program can be used to simulate a noncatalytic
 C gas-solid regeneration reaction ($\text{ZnS} + 3/2 \text{O}_2 \rightarrow$
 C $\text{ZnO} + \text{SO}_2$) in an adiabatic fixed-bed reactor.
 C Following simulation results can be used to design
 C and/or develop a tail-gas clean-up process for
 C the efficient removal of H_2S from the Claus-bed:

- C 1) O_2 breakthrough curve
- C 2) O_2 gas concentration profiles
- C 3) SO_2 gas concentration profiles
- C 4) Sorbent conversion profiles
- C 5) Sulfur loading profiles
- C 6) Gas temperature profiles
- C 7) Sorbent temperature profiles

C A shrinking core model is selected to describe the
 C kinetics of a single sorbent in the reactor.

C One dimensional heterogeneous model is used for
 C the description of the adiabatic fixed-bed reactor.

C The dimensionless governing equations are
 C integrated using the fourth order Adams-Moulton
 C predictor-corrector method.

C *****

C -----
 C NOMENCLATURE FOR THE REGENERATION PROGRAM
 C -----

C D : FIXED-BED DIAMETER (cm)
 C L : FIXED-BED LENGTH (cm)
 C BV : BED VOIDAGE (DIMENSIONLESS)
 C R : SORBENT RADIUS (cm)
 C SBDEN : SORBENT BULK DENSITY (g/cm³)
 C BVOL : BED VOLUME (cm³)
 C W : SORBENT CHARGE FOR $\text{ZNS}/\text{AL}_2\text{O}_3$ (g)
 C WSOB : SORBENT CHARGE FOR ZNS (g)
 C TEM : OPERATING TEMPERATURE (K)
 C P : OPERATING PRESSURE (atm)
 C U : SUPERFICIAL GAS VELOCITY AT TEM & P (cm/h)
 C V : VOLUMETRIC GAS FLOW RATE (cm³/h)
 C Y1 : MOLE FRACTION OF O_2 (dimensionless)
 C RG : GAS CONSTANT (cm³ atm/K mol)
 C CABO : INITIAL CONC. OF O_2 (mol/cm³)
 C CBO : INITIAL CONC. OF ZNS (mol/cm³)
 C DELH : HEAT OF REACTION AT TEM (cal/mol)
 C CYLEN : LENGTH OF A CYLINDRICAL SORBENT (cm)
 C DPE : EQUIVALENT SORBENT DIAMETER (cm)
 C G : GAS MASS FLOW RATE (g/h cm²)
 C TV1,TV2 : DIMENSIONLESS TEMPERATURES FOR O_2 & N_2
 C (=TEM*Boltzmann's const./characteristic
 C energy)
 C OM1,OM2 : VISCOSITY COLLISION INTEGRALS FOR O_2 & N_2
 C CALCULATED BY NEUFELD ET AL.' EQUATION

```

C          (dimensionless)
C VIS1,VIS2 : VISCOSITIES FOR O2 & N2 CALCULATED BY
C          CHAPMAN-ENSKOG EQUATION (g/cm s)
C PI12,PI21 : FACTORS USED IN WILKE'S EQUATION
C          (dimensionless)
C VISM : VISCOSITY OF THE MIXTURE CALCULATED BY
C          WILKE'S EQUATION (g/cm s)
C SIG12 : CHARACTERISTIC LENGTH (Angstroms)
C TV3 : DIMENSIONLESS TEMPERATURE USED IN OMD
C OMD : DIFFUSION COLLISION INTEGRAL CALCULATED BY
C          NEUFELD ET AL.' EQUATION (dimensionless)
C D12 : DIFFUSION COEFFICIENT FOR BINARY GAS SYSTEM
C          (cm2/s)
C REP : PARTICLE REYNOLDS NUMBER (dimensionless)
C SC : SCHMIDT NUMBER (dimensionless)
C SH : SHERWOOD NUMBER (dimensionless)
C NU : NUSSELT NUMBER (dimensionless)
C KM : GAS-SOLID MASS TRANSFER COEFFICIENT
C          CALCULATED BY WAKAO & FUNAZKRI'S EQUATION
C          (cm/h)
C H : GAS-SOLID HEAT TRANSFER COEFFICIENT
C          CALCULATED BY GLIDDON & CRANFIELD'S
C          EQUATION (cal/cm2 h K)
C DK : KNUDSEN DIFFUSIVITY (cm2/s)
C DC : COMBINED DIFFUSIVITY (cm2/s)
C DE1 : EFFECTIVE DIFFUSIVITY OF O2 WITHIN THE
C          SORBENT (cm2/h)
C CPG1,CPG2 : HEAT CAPACITIES FOR O2 & N2 (cal/g K)
C CPGM : AVERAGE HEAT CAPACITY OF GAS (cal/g K)
C CPS1,CPS2 : HEAT CAPACITIES FOR ZNS & AL2O3 (cal/g K)
C CPSM : AVERAGE HEAT CAPACITY OF SORBENT (cal/g K)

```

```

C -----
C ***** MAIN REGENERATION PROGRAM *****

```

```

DIMENSION XRV(251)
REAL L,M1,M2,M12,KM,KS,NU

```

```

COMMON /COM1/ INUM
COMMON /COM2/ FC2
COMMON /COM3/ FC1
COMMON /COM4/ FC3, FC4
COMMON /COM5/ FULS
COMMON /COM6/ FCRBV
COMMON /COM7/ FCBTA1, FCBTA3, FCBTA2, DE1, R
COMMON /COM8/ CABPPM
COMMON /COM9/ WSO2PM

```

```

C ----- LIST AND COMPUTATION OF INPUT DATA (FOR MODEL
C          PARAMETERS AND SECONDARY PARAMETERS)

```

```

D = 4.09
L = 19.48
BV = 0.4

```

R = 0.1588
 SBDEN = 1.121

BVOL = 3.1416*D**2*L/4.
 W = BVOL*SBDEN

WSOB = 0.5*W
 TEM = 700.
 P = 1.6

USTPFM = 0.3*33.335
 USTPCH = USTPFM*0.00508*100.*3600.
 U = USTPCH*(TEM/298.)*(1./P)
 V = U*3.1416*D**2/4.

Y1 = 0.025
 RG = 82.06
 CABPPM = Y1*(1.E6)

CABO = Y1*P/RG/TEM
 AVEX = 0.7657
 CBO = AVEX*0.5*(SBDEN/(1.-BV))/81.38

B = 0.667

DELH = -109000. + (11.4+7.7-12.81-1.5*8.27)*
 * (TEM - 298.)+((0.00145+0.0053-0.00095-
 * 1.5*0.000258)/2.)*(TEM**2-298.**2)
 * +(182400.-194600.-1.5*187700.)*(1./TEM -
 * 1./298.)-(0.00000083/3.)*(TEM**3 - 298.**3)

CYLEN = 0.9525
 DPE = (2.*R*CYLEN + 2.*R**2)**0.5
 M1 = 32.
 M2 = 28.02
 G = (P/RG/TEM)*(M1*Y1 + M2*(1. - Y1))*U

TV1 = TEM/106.7
 AA = 1.16145
 BB = 0.14874
 CC = 0.52487
 DD = 0.7732
 EE = 2.16178
 FF = 2.43787

OM1 = AA*TV1**(-BB)+CC*(EXP(-DD*TV1))+EE*
 * (EXP(-FF*TV1))
 VIS1 = (2.6693E-5)*((M1*TEM)**0.5)/3.467**2/OM1

TV2 = TEM/71.4
 OM2 = AA*TV2**(-BB)+CC*(EXP(-DD*TV2))+EE*
 * (EXP(-FF*TV2))
 VIS2 = (2.6693E-5)*((M2*TEM)**0.5)/(3.798**2)/OM2

PI12 = (1.+((VIS1/VIS2)**0.5)*(M2/M1)**0.25)**2 /
 * (8.*(1.+(M1/M2)))**0.5
 PI21 = PI12*VIS2*M1/VIS1/M2

```

VISM = Y1*VIS1/(Y1+(1.-Y1)*PI12) +
*      (1.-Y1)*VIS2/((1.-Y1)+Y1*PI21)

M12 = 2./(1./M1 + 1./M2)
SIG12 = (3.467+3.798)/2.
TV3 = TEM/(106.7*71.4)**0.5
OMD = 1.06036/TV3**0.1561 + 0.193/EXP(0.47635*TV3)
*      + 1.03587/EXP(1.52996*TV3)
*      + 1.76474/EXP(3.89411*TV3)
D12 = 0.00266*TEM**1.5/(P*1.0133)/(M12**0.5)/
*      (SIG12**2)/OMD

REP = DPE*G/3600./VISM
SC = VISM/D12/(G/U)
SH = 2. + 1.1*(SC**(1./3.))*(REP**0.6)
NU = 0.36*REP**0.94

KM = 3600.*SH*D12/DPE

H = 3600.*NU*((0.0528*Y1 + 0.0498*(1.-Y1))/418.7)/DPE

DK = (9.7E3)*(1.156E-6)*(TEM/M1)**0.5
DC = DK*D12/(DK + D12)
DE1 = 3600.*DC*(1.-((SBDEN/(1.-BV))/4.653))**2

CPG1 = (8.27+0.000258*TEM-187700./TEM**2)/32.
CPG2 = (6.5 + 0.001*TEM)/28.02
CPGM = Y1 * CPG1 + (1.-Y1)*CPG2

CPS1 = (22.08 + 0.008971*TEM - 522500./(TEM**2))/
*      101.963
CPS2 = (12.81+0.00095*TEM - 194600./TEM**2)/97.44
CPSM = 0.5*CPS1 + 0.5*CPS2

KS = 4.E8
FULS = 0.3284
ASV = 2.*(1.-BV)/R

```

C ----- COMPUTATION OF FACTORS IN FUNCTION BETA

```

FCBTA1 = 2.*(1.-BV)/(U/L)
FCBTA2 = R/KM
FCBTA3 = R/(KS*CB0)

```

C ----- COMPUTATION OF A FACTOR IN FUNCTION RBV

```

FCRBV = (U/L)*B*CAB0/(1.-BV)

```

C -----

```

TIMX = WSOB/97.44/B/(CAB0*U*3.1415/4.*D**2)
WRITE (6,15) TIMX
15  FORMAT(/2X,' TIME NEEDED TO REGENERATE A FULLY'
*      /2X,' SULFIDED BED = ',E10.2,' HR')

```

```

C ----- COMPUTATION OF FACTORS IN DIMENSIONLESS
C           GOVERNING EQUATIONS

FC1 = CAB0*B*U/(CB0*L*(1.-BV))
FC2 = H*ASV*L/(G*CPGM)
FC3 = -DELH/(SBDEN/(1.-BV))/CPSM/TEM
FC4 = H*ASV/(1.-BV)/(SBDEN/(1.-BV))/CPSM

C ----- TIME AND Z STEP SIZES FOR THE INTEGRATION OF
C           DIMENSIONLESS GOVERNING EQUATIONS

DLT = 0.002
INUM = 250
DLZ = 1./INUM
INUM = INUM+1

C -----

TBGIN = 0.002
TINT = 0.002
TEND = 0.002

BBGIN = 0.1
BINT = 0.1
BEND = 1.

C -----

WRITE (6,28)
28  FORMAT (// '      ENTER WANTED EXIT SO2 PPM: ')
READ (5,*) WSO2PM

C ----- READ IN THE SULFIDATION CONVERSION FROM A
C           PREVIOUS CYCLE AND REVERSE THE ORDER OF
C           THE CONVERSION)

CALL RVCONV(XRV)

C ----- PROVIDE INITIAL SULFUR LOADING FOR
C           REGENERATION

CALL RGSLDI(XRV)

C ----- ENTER THE TIME FOR REGENERATION

CALL RGTIME(TBGIN,TINT,TEND)

C ----- CALL ADAMS-MOULTON 4TH ORDER METHOD FOR
C           INTEGRATION

CALL AMPC(DLZ,DLT,TBGIN,TINT,TEND,XRV,BBGIN,BINT,
*         BEND)

```

STOP
END

C ***** END OF MAIN *****

C ***** SUBROUTINE RVCONV *****

```

SUBROUTINE RVCONV(XSR)
DIMENSION XSR(251)
CHARACTER*8 DATNAM
COMMON /COM1/ INUM

WRITE (6,20)
20  FORMAT (/ '      ENTER SORBENT CONVERSION      '
*      / '      (AT SULFIDATION BREAKTHROUGH TIME) '
*      / '      DATA FILE NAME: ' )
READ (5,21) DATNAM
21  FORMAT (8A)
OPEN (UNIT = 13, FILE = DATNAM)

DO 23 I = 1, INUM
23  READ (13,28) XSR(I)
28  FORMAT(E18.9)

DO 25 I = 1, INT(INUM/2)
    TEM = XSR(INUM-I+1)
    XSR(INUM-I+1) = XSR(I)
    XSR(I) = TEM
25  CONTINUE

REWIND (13)
CLOSE (13)

RETURN
END

```

C ***** SUBROUTINE RGSLDI *****

```

SUBROUTINE RGSLDI(XRV)

DIMENSION XRV(251), Z(51)
COMMON /COM1/ INUM
COMMON /COM5/ FULS

OPEN(14,FILE='SLH22.DAT',STATUS='NEW')
WRITE(14,80)

DO 81 I = 1,51
81  Z(I) = 0.02*(I-1)

I1 = 1
DLZ = 1./(INUM-1)

DO 83 I2 = 1,51

```

```

      I3 = I1 + (INUM-1)/50.*(I2-1)
      WRITE(14,85) Z(I2), XRV(I3)*FULS
83  CONTINUE

85  FORMAT (18X,F9.3,6X,E12.5)
80  FORMAT(// '          INITIAL SULFUR LOADING'
*      ' FOR REGENERATION:'
*      // '          Z'
*      '          SULFUR LOADING'//)

      CLOSE(14)
      RETURN
      END

C ***** SUBROUTINE RGTIME *****

      SUBROUTINE RGTIME(TBGIN,TINT,TEND)
      COMMON /COM1/ INUM

39  WRITE (6,35)
35  FORMAT(/ '          ENTER BEGINNING, INTERVAL AND ENDING'
* / '          TIME FOR REGENERATION SIMULATION (hr):')
      READ (5,*) TBGIN,TINT,TEND

      IF((TBGIN.GT.TEND).OR.(TINT.GT.TEND)) THEN
          WRITE (6,36)
36  FORMAT ('OOOOOPS ! ENTER AGAIN !')
          GO TO 39
      END IF

      IF(ABS(TBGIN).LE.1.E-2) TBGIN = TINT

      RETURN
      END

C ***** SUBROUTINE AMPC *****

C ----- USE ADAMS-MOULTON 4TH ORDER METHOD FOR THE
C          INTEGRATION OF DIMENSIONLESS GOVERNING EQNS.

      SUBROUTINE AMPC(DLZ,DLT,TBGIN,TINT,TEND,XRV,BBGIN,
*          BINT,BEND)

      LOGICAL WTIME

      DIMENSION XRV(251)
      DIMENSION Z(251),TG(251),TS(251),CAB(251),X(251),
*          WRX(251),WSLOD(251)
      DIMENSION TS1(251),TG1(251),X1(251),CAB1(251)
      DIMENSION TS2(251),TG2(251),X2(251),CAB2(251)
      DIMENSION TS3(251),TG3(251),X3(251),CAB3(251)

      DIMENSION REGCAB(12550),REGX(12550),REGSLD(12550),
*          REGTG(12550),REGTS(12550),PPMEXT(12550),
*          PPMSO2(12550)

```



```

DIMENSION IBPNT(10),TGIMSI(10,50),TSIMSI(10,50),
*          BTG(500),BTS(500)

COMMON /COM1/ INUM
COMMON /COM2/ FC2
COMMON /COM3/ FC1
COMMON /COM4/ FC3,FC4
COMMON /COM5/ FULS
COMMON /COM6/ FCRBV
COMMON /COM7/ FCBTA1,FCBTA3,FCBTA2,DE1,R
COMMON /COM8/ CABPPM
COMMON /COM9/ WSO2PM

C -----
OPEN(15,FILE='WHX22')
OPEN(17,FILE='WHD22')
C -----

WTIME = .FALSE.

C -----

NBLIN = INT((BEND-BBGIN)/BINT*1.001) + 1
IBPNT(1) = INT((INUM-1)*BBGIN*1.0001) + 1
DO 500 IBED = 1,NBLIN-1
500     IBPNT(IBED+1) = INT((INUM-1)*(BBGIN+BINT*
*          IBED)*1.0001) + 1

NT = 1
NTIME = 50
BTBGIN = TEND/NTIME
BDEPSI = 0.5*BTBGIN

C -----
C
EPSI = 1.E-50
EPS = 0.5*DLT

T = 0.
PPMEXT(1) = 0.
PPMSO2(1) = 0.

Z(1) = 0.

DO 41 I = 1, INUM-1

    Z(I+1) = Z(I) + DLZ

41  CONTINUE

C ----- INITIAL CONDITIONS FOR THE INTEGRATION OF
C          DIMENSIONLESS GOVERNING EQUATIONS

CAB(1) = 1.
TG(1) = 1.

```

```

DO 42 I = 1, INUM

      X(I) = 0.
      TS(I) = 1.

42  CONTINUE

C -----
      WRITE (6,300)
300  FORMAT(//'          PLEASE, WAIT FOR SIMULATION RESULTS'
* ' !',)

C -----

C ----- COMPUTE AT THE FOLLOWING GRID POINT:
C          (i,j) = (2,1)

      CABSE = CAB(1) + DLZ*FN1(X(1),CAB(1))
      IF(CABSE.LT.EPSI) CABSE = EPSI
      IF(ABS(CABSE).GT.1.0) CABSE = 1.0
      TGSE = TG(1) + DLZ*FN2(TS(1),TG(1))

      CAB(2) = CAB(1) + 0.5*DLZ*(FN1(X(1),CAB(1))
*          +FN1(X(2),CABSE))
      TG(2) = TG(1) + 0.5*DLZ*(FN2(TS(1),TG(1))
*          + FN2(TS(2),TGSE))

C ----- COMPUTE AT: (i,j) = (3,1) & (4,1)

DO 51 I = 3,4

      CABPD = CAB(I-2)+2.0*DLZ*FN1(X(I-1),CAB(I-1))
      TGPD = TG(I-2)+2.0*DLZ*FN2(TS(I-1),TG(I-1))
      IF(ABS(CABPD).LE.EPSI) CABPD = EPSI

      CAB(I) = CAB(I-1)+0.5*DLZ*(FN1(X(I-1),CAB(I-1))
*          + FN1(X(I),CABPD))
      TG(I) = TG(I-1)+0.5*DLZ*(FN2(TS(I-1),TG(I-1))
*          + FN2(TS(I),TGPD))
      IF(ABS(CAB(I)).LT.EPSI) CAB(I) = EPSI

51  CONTINUE

C ----- COMPUTE AT: (i,j) = FROM (5,1) TO (INUM,1)

DO 52 I = 5,INUM

      CABPD = CAB(I-1)+(DLZ/24.)*(55.*FN1(X(I-1),
*          CAB(I-1))-59.*FN1(X(I-2),CAB(I-2))+
*          37.*FN1(X(I-3),CAB(I-3))-9.*
*          FN1(X(I-4),CAB(I-4)))
      TGPD = TG(I-1)+(DLZ/24.)*(55.*FN2(TS(I-1),TG(I-1))
*          -59.*FN2(TS(I-2),TG(I-2))+37.*FN2(TS(I-3),
*          TG(I-3))-9.*FN2(TS(I-4),TG(I-4)))

```

```
IF(ABS(CABPD).LE.EPSI) CABPD = EPSI
```

```
CAB(I) = CAB(I-1)+(DLZ/24.)*(9.*FN1(X(I),CABPD)
*      +19.*FN1(X(I-1),CAB(I-1))-5.*FN1(X(I-2),
*      CAB(I-2))+FN1(X(I-3),CAB(I-3)))
TG(I) = TG(I-1)+(DLZ/24.)*(9.*FN2(TS(I),TGPD)
*      +19.*FN2(TS(I-1),TG(I-1))-5.*FN2(TS(I-2),
*      TG(I-2))+FN2(TS(I-3),TG(I-3)))
IF(ABS(CAB(I)).LT.EPSI) CAB(I) = EPSI
```

```
52 CONTINUE
```

```
C -----
C ----- GOING TO THE NEXT TIME STEP
C ----- COMPUTE AT: (i,j) = (1,2)
```

```
XSE = X(1) + FN3(X(1),CAB(1))*DLT
IF(XSE.LT.EPSI) XSE = EPSI
IF(XSE.GT.1.) XSE = 1.0
TSSE = TS(1) + FN4(TS(1),TG(1),X(1),CAB(1))*DLT

XCT = X(1)+0.5*DLT*(FN3(X(1),CAB(1))+FN3(XSE,CAB(1)))
TSCT = TS(1) + 0.5*DLT*(FN4(TS(1),TG(1),X(1),CAB(1))
*      +FN4(TSSE,TG(1),XSE,CAB(1)))
IF(XCT.LT.EPSI) XCT = EPSI
IF(XCT.GT.1.) XCT = 1.0

X1(1) = X(1)
TS1(1) = TS(1)
X(1) = XCT
IF(X(1).GT.XRV(1)) X(1) = 1.
TS(1) = TSCT
```

```
C ----- COMPUTE AT: (i,j) = (2,2)
```

```
TSSE = TS(2) + DLT*FN4(TS(2),TG(2),X(2),CAB(2))
XSE = X(2) + DLT*FN3(X(2),CAB(2))
CABSE = CAB(1) + DLZ*FN1(X(1),CAB(1))
IF(ABS(CABSE).LT.EPSI) CABSE = EPSI
IF(ABS(XSE).LT.EPSI) XSE = EPSI
TGSE = TG(1) + DLZ*FN2(TS(1),TG(1))

TSCT = TS(2) + 0.5*DLT*(FN4(TS(2),TG(2),X(2),CAB(2))
*      +FN4(TSSE,TGSE,XSE,CABSE))
XCT = X(2)+0.5*DLT*(FN3(X(2),CAB(2))+FN3(XSE,CABSE))
CABCT = CAB(1)+0.5*DLZ*(FN1(X(1),CAB(1))
*      +FN1(XSE,CABSE))

IF(ABS(CABCT).LT.EPSI) CABCT = EPSI
IF(ABS(XCT).LT.EPSI) XCT = EPSI
TGCT = TG(1)+0.5*DLZ*(FN2(TS(1),TG(1))+
*      FN2(TSSE,TGSE))

X1(2) = X(2)
TS1(2) = TS(2)
```

```

CAB1(2) = CAB(2)
TG1(2) = TG(2)
X(2) = XCT
IF(X(2).GT.XRV(2)) X(2)=1.
TS(2) = TSCT
CAB(2) = CABCT
TG(2) = TGCT

```

C ----- COMPUTE AT: (i,j) = (3,2) & (4,2)

```

DO 53 I = 3,4
  XSE = X(I) + DLT*FN3(X(I),CAB(I))
  TSSE = TS(I) + DLT*FN4(TS(I),TG(I),X(I),CAB(I))
  IF(ABS(XSE).LT.EPSI) XSE = EPSI

  TGPDP = TG(I-2)+2.0*DLZ*FN2(TS(I-1),TG(I-1))
  CABPDP = CAB(I-2)+2.0*DLZ*FN1(X(I-1),CAB(I-1))
  IF(ABS(CABPDP).LT.EPSI) CABPDP = EPSI

  XCT = X(I)+0.5*DLT*(FN3(X(I),CAB(I))+
*      FN3(XSE,CABPDP))
  TSCT = TS(I) + 0.5*DLT*(FN4(TS(I),TG(I),X(I),
*      CAB(I))+FN4(TSSE,TGPDP,XSE,CABPDP))
  IF(ABS(XCT).LT.EPSI)XCT=EPSI
  CABCT = CAB(I-1) + 0.5*DLZ*(FN1(X(I-1),
*      CAB(I-1))+FN1(XCT,CABPDP))
  IF(ABS(CABCT).LT.EPSI) CABCT = EPSI
  TGCT = TG(I-1)+0.5*DLZ*(FN2(TS(I-1),TG(I-1))
*      +FN2(TSCT,TGPDP))

  X1(I) = X(I)
  TS1(I) = TS(I)
  CAB1(I) = CAB(I)
  TG1(I) = TG(I)
  X(I) = XCT
  IF(X(I).GT.XRV(I)) X(I)=1.
  TS(I) = TSCT
  CAB(I) = CABCT
  TG(I) = TGCT

```

53 CONTINUE

C ----- COMPUTE AT: (i,j) = FROM (5,2) TO (INUM,2)

```

DO 54 I = 5,INUM

  XSE = X(I)+DLT*FN3(X(I),CAB(I))
  TSSE = TS(I)+DLT*FN4(TS(I),TG(I),X(I),CAB(I))
  IF(ABS(XSE).LT.EPSI) XSE = EPSI

  TGPDP = TG(I-1)+(DLZ/24.)*(55.*FN2(TS(I-1),TG(I-1))
*      -59.*FN2(TS(I-2),TG(I-2)) + 37.*FN2(TS(I-3),
*      TG(I-3))-9.*FN2(TS(I-4),TG(I-4)))
  CABPDP =CAB(I-1)+(DLZ/24.)*(55.*FN1(X(I-1),CAB(I-1))
*      -59.*FN1(X(I-2),CAB(I-2))+37.*FN1(X(I-3),

```

```

*      CAB(I-3))-9.*FN1(X(I-4),CAB(I-4)))
IF(ABS(CABPD).LT.EPSI) CABPD = EPSI

XCT =X(I)+0.5*DLT*(FN3(X(I),CAB(I))+FN3(XSE,CABPD))
TSCT = TS(I)+0.5*DLT*(FN4(TS(I),TG(I),X(I),CAB(I))
*      +FN4(TSSE,TGPD,XSE,CABPD))
IF(ABS(XCT).LT.EPSI) XCT = EPSI

CABCT = CAB(I-1)+(DLZ/24.)*(9.*FN1(XCT,CABPD)
*      +19.*FN1(X(I-1),CAB(I-1)) - 5.*FN1(X(I-2),
*      CAB(I-2))+FN1(X(I-3),CAB(I-3)))
IF(ABS(CABCT).LT.EPSI) CABCT = EPSI
TGCT = TG(I-1)+(DLZ/24.)*(9.*FN2(TSCT,TGPD)
*      +19.*FN2(TS(I-1),TG(I-1)) - 5.*FN2(TS(I-2),
*      TG(I-2))+FN2(TS(I-3),TG(I-3)))

X1(I) = X(I)
TS1(I) = TS(I)
CAB1(I) = CAB(I)
TG1(I) = TG(I)

X(I) = XCT
IF(X(I).GT.XRV(I)) X(I) = 1.
TS(I) = TSCT
CAB(I) = CABCT
TG(I) = TGCT

```

54 CONTINUE

C -----
C ----- GOING TO THE NEXT TIME STEP

T = T + DLT

C ----- COMPUTE AT: (i,j) = (1,3)

```

XPD = X1(1) + 2.0*DLT*FN3(X(1),CAB(1))
TSPD = TS1(1)+2.0*DLT*FN4(TS(1),TG(1),X(1),CAB(1))
IF(ABS(XPD).LT.EPSI) XPD = EPSI
XCT = X(1)+0.5*DLT*(FN3(X(1),CAB(1))+
*      FN3(XPD,CAB(1)))
TSCT = TS(1)+0.5*DLT*(FN4(TS(1),TG(1),X(1),CAB(1))
*      +FN4(TSPD,TG(1),XPD,CAB(1)))
IF(ABS(XCT).LT.EPSI)XCT=EPSI

X2(1) = X(1)
TS2(1) = TS(1)
X(1) = XCT
IF(X(1).GT.XRV(1)) X(1) = 1.
TS(1) = TSCT

```

C ----- COMPUTE AT: (i,j) = (2,3)

```

CABSE = CAB(1) + DLZ*FN1(X(1),CAB(1))
IF(ABS(CABSE).LT.EPSI) CABSE = EPSI

```

```

TGSE = TG(1) + DLZ*FN2(TS(1),TG(1))
XPD = X1(2) + 2.0*DLT*FN3(X(2),CAB(2))
TSPD = TS1(2)+2.0*DLT*FN4(TS(2),TG(2),X(2),CAB(2))
IF(ABS(XPD).LT.EPSI) XPD = EPSI
CABCT = CAB(1)+0.5*DLZ*(FN1(X(1),CAB(1))+FN1(
*   XPD,CABSE))
IF(ABS(CABCT).LT.EPSI) CABCT = EPSI
TGCT = TG(1) + 0.5*DLZ*(FN2(TS(1),TG(1))
*   + FN2(TSPD,TGSE))
XCT = X(2)+0.5*DLT*(FN3(X(2),CAB(2))+
*   FN3(XPD,CABCT))
TSCT = TS(2)+0.5*DLT*(FN4(TS(2),TG(2),X(2),CAB(2))
*   +FN4(TSPD,TGCT,XPD,CABCT))
IF(ABS(XCT).LT.EPSI)XCT=EPSI

X2(2) = X(2)
TS2(2) = TS(2)
CAB2(2) = CAB(2)
TG2(2) = TG(2)

X(2) = XCT
IF(X(2).GT.XRV(2)) X(2)=1.
TS(2) = TSCT
CAB(2) = CABCT
TG(2) = TGCT

```

C ----- COMPUTE AT: (i,j) = (3,3) & (4,3)

```

DO 55 I = 3,4
  CABPD = CAB(I-2)+2.0*DLZ*FN1(X(I-1),CAB(I-1))
  IF(ABS(CABPD).LT.EPSI) CABPD = EPSI
  TGPD = TG(I-2) + 2.0*DLZ*FN2(TS(I-1),TG(I-1))
  XPD = X1(I) + 2.0*DLT*FN3(X(I),CAB(I))
  IF(ABS(XPD).LT.EPSI) XPD=EPSI
  TSPD = TS1(I)+2.0*DLT*FN4(TS(I),TG(I),X(I),
*   CAB(I))

  CABCT = CAB(I-1)+0.5*DLZ*(FN1(X(I-1),
*   CAB(I-1))+FN1(XPD,CABPD))
  IF(ABS(CABCT).LT.EPSI) CABCT = EPSI
  TGCT = TG(I-1)+0.5*DLZ*(FN2(TS(I-1),TG(I-1))
*   +FN2(TSPD,TGPD))
  XCT = X(I) + 0.5*DLT*(FN3(X(I),CAB(I))
*   + FN3(XPD,CABCT))
  IF(ABS(XCT).LT.EPSI)XCT=EPSI
  TSCT = TS(I) + 0.5*DLT*(FN4(TS(I),TG(I),X(I),
*   CAB(I))+ FN4(TSPD,TGCT,XPD,CABCT))

  X2(I) = X(I)
  TS2(I) = TS(I)
  CAB2(I) = CAB(I)
  TG2(I) = TG(I)

  X(I) = XCT
  IF(X(I).GT.XRV(I)) X(I)=1.

```

```

    TS(I) = TSCT
    CAB(I) = CABCT
    TG(I) = TGCT

```

55 CONTINUE

C ----- COMPUTE AT: (i,j) = FROM (5,3) TO (INUM,3)

```

DO 56 I=5,INUM
  CABPD =CAB(I-1)+(DLZ/24.)*(55.*FN1(X(I-1),CAB(I-1))
*      -59.*FN1(X(I-2),CAB(I-2))+37.*FN1(X(I-3),
*      CAB(I-3))-9.*FN1(X(I-4),CAB(I-4)))
  IF(ABS(CABPD).LT.EPSI) CABPD = EPSI
  TGPD = TG(I-1)+(DLZ/24.)*(55.*FN2(TS(I-1),TG(I-1))
*      -59.*FN2(TS(I-2),TG(I-2))+37.*FN2(TS(I-3),
*      TG(I-3))-9.*FN2(TS(I-4),TG(I-4)))
  XPD = X1(I)+2.0*DLT*FN3(X(I),CAB(I))
  IF(ABS(XPD).LT.EPSI) XPD = EPSI
  TSPD = TS1(I)+2.0*DLT*FN4(TS(I),TG(I),X(I),CAB(I))

  CABCT = CAB(I-1)+(DLZ/24.)*(9.*FN1(XPD,CABPD)
*      +19.*FN1(X(I-1),CAB(I-1))-5.*FN1(X(I-2),
*      CAB(I-2))+FN1(X(I-3),CAB(I-3)))
  IF(ABS(CABCT).LT.EPSI) CABCT = EPSI
  TGCT = TG(I-1)+(DLZ/24.)*(9.*FN2(TSPD,TGPD)
*      +19.*FN2(TS(I-1),TG(I-1))
*      -5.*FN2(TS(I-2),TG(I-2))+FN2(TS(I-3),
*      TG(I-3)))
  XCT = X(I)+0.5*DLT*(FN3(X(I),CAB(I))+
*      FN3(XPD,CABCT))
  IF(ABS(XCT).LT.EPSI) XCT = EPSI
  TSCT = TS(I)+0.5*DLT*(FN4(TS(I),TG(I),X(I),CAB(I))
*      +FN4(TSPD,TGCT,XPD,CABCT))

```

```

X2(I)=X(I)
TS2(I)=TS(I)
CAB2(I) = CAB(I)
TG2(I) = TG(I)

```

```

X(I)= XCT
IF(X(I).GT.XRV(I)) X(I)=1.
TS(I)= TSCT
CAB(I)= CABCT
TG(I)= TGCT

```

56 CONTINUE

C -----
C ----- GOING TO THE NEXT TIME STEP

T = T + DLT

C ----- COMPUTE AT: (i,j) = (1,4)

```

XPD = X2(1) + 2.0*DLT*FN3(X(1),CAB(1))

```

```

TSPD = TS2(1) + 2.0*DLT*FN4(TS(1),TG(1),X(1),CAB(1))
IF(ABS(XPD).LT.EPSI) XPD = EPSI
XCT = X(1)+0.5*DLT*(FN3(X(1),CAB(1))+FN3(XPD,CAB(1)))
TSCT = TS(1) + 0.5*DLT*(FN4(TS(1),TG(1),X(1),CAB(1))
*      +FN4(TSPD,TG(1),XPD,CAB(1)))
IF(ABS(XCT).LT.EPSI) XCT = EPSI

X3(1) = X(1)
TS3(1) = TS(1)
X(1) = XCT
IF(X(1).GT.XRV(1)) X(1) = 1.
TS(1) = TSCT

```

C ----- COMPUTE AT: (i,j) = (2,4)

```

CABSE = CAB(1) + DLZ*FN1(X(1),CAB(1))
IF(ABS(CABSE).LT.EPSI) CABSE = EPSI
TGSE = TG(1) + DLZ*FN2(TS(1),TG(1))
XPD = X2(2) + 2.0*DLT*FN3(X(2),CAB(2))
TSPD = TS2(2) + 2.0*DLT*FN4(TS(2),TG(2),X(2),CAB(2))
IF(ABS(XPD).LT.EPSI) XPD = EPSI

CABCT = CAB(1) + 0.5*DLZ*(FN1(X(1),CAB(1)) +
*      FN1(XPD,CABSE))
IF(ABS(CABCT).LT.EPSI) CABCT = EPSI
TGCT = TG(1)+0.5*DLZ*(FN2(TS(1),TG(1))+
*      FN2(TSPD,TGSE))
XCT = X(2)+0.5*DLT*(FN3(X(2),CAB(2))+FN3(XPD,CABCT))
TSCT = TS(2) + 0.5*DLT*(FN4(TS(2),TG(2),X(2),CAB(2))
*      +FN4(TSPD,TGCT,XPD,CABCT))
IF(ABS(XCT).LT.EPSI) XCT = EPSI

X3(2) = X(2)
TS3(2) = TS(2)
CAB3(2) = CAB(2)
TG3(2) = TG(2)

X(2) = XCT
IF(X(2).GT.XRV(2)) X(2)=1.
TS(2) = TSCT
CAB(2) = CABCT
TG(2) = TGCT

```

C ----- COMPUTE AT: (i,j) = (3,4) & (4,4)

DO 57 I = 3,4

```

CABPD = CAB(I-2)+2.0*DLZ*FN1(X(I-1),CAB(I-1))
IF(ABS(CABPD).LT.EPSI) CABPD = EPSI
TGPD = TG(I-2) + 2.0*DLZ*FN2(TS(I-1),TG(I-1))
XPD = X2(I) + 2.0*DLT*FN3(X(I),CAB(I))
IF(ABS(XPD).LT.EPSI) XPD = EPSI
TSPD = TS2(I) + 2.0*DLT*FN4(TS(I),TG(I),X(I),CAB(I))

CABCT = CAB(I-1)+0.5*DLZ*(FN1(X(I-1),CAB(I-1))+

```



```

*          FN1(XPD,CABPD))
IF(ABS(CABCT).LT.EPSI) CABCT = EPSI
TGCT = TG(I-1)+0.5*DLZ*(FN2(TS(I-1),TG(I-1))+
*          FN2(TSPD,TGPD))
XCT = X(I)+0.5*DLT*(FN3(X(I),CAB(I))+FN3(XPD,CABCT))
IF(ABS(XCT).LT.EPSI) XCT =EPSI
TSCT = TS(I)+0.5*DLT*(FN4(TS(I),TG(I),X(I),CAB(I))
*          + FN4(TSPD,TGCT,XPD,CABCT))

X3(I) = X(I)
TS3(I) = TS(I)
CAB3(I) = CAB(I)
TG3(I) = TG(I)

X(I) = XCT
IF(X(I).GT.XRV(I)) X(I) = 1.
TS(I) = TSCT
CAB(I) = CABCT
TG(I) = TGCT

```

57 CONTINUE

C ----- COMPUTE AT: (i,j) = FROM (5,4) TO (INUM,4)

DO 58 I = 5,INUM

```

CABPD =CAB(I-1)+(DLZ/24.)*(55.*FN1(X(I-1),CAB(I-1))
*          -59.*FN1(X(I-2),CAB(I-2))+37.*FN1(X(I-3),
*          CAB(I-3))-9.*FN1(X(I-4),CAB(I-4)))
IF(ABS(CABPD).LT.EPSI) CABPD = EPSI
TGPD = TG(I-1)+(DLZ/24.)*(55.*FN2(TS(I-1),TG(I-1))
*          -59.*FN2(TS(I-2),TG(I-2))+37.*FN2(TS(I-3),
*          TG(I-3))-9.*FN2(TS(I-4),TG(I-4)))
XPD = X2(I)+2.0*DLT*FN3(X(I),CAB(I))
IF(ABS(XPD).LT.EPSI) XPD=EPSI
TSPD = TS2(I)+2.0*DLT*FN4(TS(I),TG(I),X(I),CAB(I))

CABCT = CAB(I-1)+(DLZ/24.)*(9.*FN1(XPD,CABPD)
*          +19.*FN1(X(I-1),CAB(I-1))
*          -5.*FN1(X(I-2),CAB(I-2))+
*          FN1(X(I-3),CAB(I-3)))
IF(ABS(CABCT).LT.EPSI) CABCT = EPSI
TGCT = TG(I-1)+(DLZ/24.)*(9.*FN2(TSPD,TGPD)
*          +19.*FN2(TS(I-1),TG(I-1))
*          -5.*FN2(TS(I-2),TG(I-2))+
*          FN2(TS(I-3),TG(I-3)))
XCT = X(I)+0.5*DLT*(FN3(X(I),CAB(I))+
*          FN3(XPD,CABCT))
IF(ABS(XCT).LT.EPSI) XCT = EPSI
TSCT = TS(I)+0.5*DLT*(FN4(TS(I),TG(I),X(I),CAB(I))
*          +FN4(TSPD,TGCT,XPD,CABCT))

X3(I) = X(I)
TS3(I) = TS(I)
CAB3(I) = CAB(I)

```

```
TG3(I) = TG(I)
```

```
X(I) = XCT
IF(X(I).GT.XRV(I)) X(I) = 1.
TS(I) = TSCT
CAB(I) = CABCT
TG(I) = TGCT
```

```
58 CONTINUE
```

```
C -----
C ----- GOING TO THE NEXT TIME STEP
```

```
T = T + DLT
```

```
C ----- COMPUTE UP TO THE FINAL TIME STEP
C
```

```
JSTP = INT(TEND/DLT) + 2
I1 = 0
I5 = 2
DO 100 J = 5, JSTP
```

```
C ----- COMPUTE AT: i = 1
```

```
XPD = X(1)+(DLT/24.)*(55.*FN3(X(1),CAB(1))
* -59.*FN3(X3(1),CAB(1))+37.*FN3(X2(1),CAB(1))
* -9.*FN3(X1(1),CAB(1)))
TSPD = TS(1)+(DLT/24.)*(55.*
* FN4(TS(1),TG(1),X(1),CAB(1))
* -59.*FN4(TS3(1),TG(1),X3(1),CAB(1))
* +37.*FN4(TS2(1),TG(1),X2(1),CAB(1))
* -9.*FN4(TS1(1),TG(1),X1(1),CAB(1)))
IF(ABS(XPD).LT.EPSI) XPD=EPSI
```

```
XCT = X(1)+(DLT/24.)*(9.*FN3(XPD,CAB(1))+19.*
* FN3(X(1),CAB(1))-5.*FN3(X3(1),CAB(1))+
* FN3(X2(1),CAB(1)))
TSCT = TS(1)+(DLT/24.)*(9.*FN4(TSPD,TG(1),XPD,CAB(1))
* +19.*FN4(TS(1),TG(1),X(1),CAB(1))
* -5.*FN4(TS3(1),TG(1),X3(1),
* CAB(1))+FN4(TS2(1),TG(1),X2(1),CAB(1)))
IF(ABS(XCT).LT.EPSI) XCT = EPSI
```

```
X1(1) = X2(1)
X2(1) = X3(1)
TS1(1) = TS2(1)
TS2(1) = TS3(1)
```

```
X3(1) = X(1)
TS3(1) = TS(1)
X(1) = XCT
IF(X(1).GT.XRV(1)) X(1) = 1.
TS(1) = TSCT
```

```
C ----- COMPUTE AT: i = 2
```

```

CABSE = CAB(1)+DLZ*FN1(X(1),CAB(1))
IF(ABS(CABSE).LT.EPSI) CABSE=EPSI
TGSE = TG(1)+DLZ*FN2(TS(1),TG(1))
XPD = X(2)+(DLT/24.)*(55.*FN3(X(2),CAB(2))
*      -59.*FN3(X3(2),CAB3(2))
*      +37.*FN3(X2(2),CAB2(2))-9.*FN3(X1(2),CAB1(2)))
TSPD = TS(2)+(DLT/24.)*(55.*FN4(TS(2),TG(2),X(2),
*      CAB(2))-59.*FN4(TS3(2),TG3(2),X3(2),CAB3(2))
*      +37.*FN4(TS2(2),TG2(2),X2(2),CAB2(2))-9.*
*      FN4(TS1(2),TG1(2),X1(2),CAB1(2)))
IF(ABS(XPD).LT.EPSI) XPD = EPSI

CABCT = CAB(1)+0.5*DLZ*(FN1(X(1),CAB(1))+
*      FN1(XPD,CABSE))
IF(ABS(CABCT).LT.EPSI) CABCT = EPSI
TGCT = TG(1)+0.5*DLZ*(FN2(TS(1),TG(1))+
*      FN2(TSPD,TGSE))
XCT = X(2)+(DLT/24.)*(9.*FN3(XPD,CABCT)+19.*
*      FN3(X(2),CAB(2))-5.*FN3(X3(2),CAB3(2))+
*      FN3(X2(2),CAB2(2)))
TSCT = TS(2)+(DLT/24.)*(9.*FN4(TSPD,TGCT,XPD,CABCT)
*      +19.*FN4(TS(2),TG(2),X(2),CAB(2))
*      -5.*FN4(TS3(2),TG3(2),X3(2),CAB3(2))
*      +FN4(TS2(2),TG2(2),X2(2),CAB2(2)))
IF(ABS(XCT).LT.EPSI) XCT = EPSI

X1(2) = X2(2)
X2(2) = X3(2)
TS1(2) = TS2(2)
TS2(2) = TS3(2)
C      CAB1(2) = CAB2(2)
C      CAB2(2) = CAB3(2)
TG1(2) = TG2(2)
TG2(2) = TG3(2)

X3(2) = X(2)
TS3(2) = TS(2)
C      CAB3(2) = CAB(2)
TG3(2) = TG(2)

X(2) = XCT
IF(X(2).GT.XRV(2)) X(2) =1.
TS(2) = TSCT
CAB(2) = CABCT
TG(2) = TGCT

C ----- COMPUTE AT: i = 3 & 4

DO 60 I = 3,4

CABPD = CAB(I-2)+2.*DLZ*FN1(X(I-1),CAB(I-1))
IF(ABS(CABPD).LT.EPSI) CABPD = EPSI
TGPD = TG(I-2)+2.*DLZ*FN2(TS(I-1),TG(I-1))
XPD = X(I)+(DLT/24.)*(55.*FN3(X(I),CAB(I))

```

```

*      -59.*FN3(X3(I),CAB3(I))
*      +37.*FN3(X2(I),CAB2(I))-9.*FN3(X1(I),CAB1(I)))
TSPD = TS(I)+(DLT/24.)*(55.*FN4(TS(I),TG(I),X(I),
*      CAB(I))-59.*FN4(TS3(I),TG3(I),X3(I),CAB3(I))
*      +37.*FN4(TS2(I),TG2(I),X2(I),CAB2(I))-9.*
*      FN4(TS1(I),TG1(I),X1(I),CAB1(I)))
IF(ABS(XPD).LT.EPSI) XPD = EPSI

CABCT = CAB(I-1)+0.5*DLZ*(FN1(X(I-1),CAB(I-1))+
*      FN1(XPD,CABPD))
IF(ABS(CABCT).LT.EPSI) CABCT = EPSI
TGCT = TG(I-1)+0.5*DLZ*(FN2(TS(I-1),TG(I-1))+
*      FN2(TSPD,TGPD))
XCT = X(I)+(DLT/24.)*(9.*FN3(XPD,CABCT)+19.*
*      FN3(X(I),CAB(I))-5.*FN3(X3(I),CAB3(I))+
*      FN3(X2(I),CAB2(I)))
IF(ABS(XCT).LT.EPSI) XCT = EPSI
TSCT = TS(I)+(DLT/24.)*(9.*FN4(TSPD,TGCT,XPD,CABCT)
*      +19.*FN4(TS(I),TG(I),X(I),CAB(I))
*      -5.*FN4(TS3(I),TG3(I),X3(I),CAB3(I))
*      +FN4(TS2(I),TG2(I),X2(I),CAB2(I)))

X1(I) = X2(I)
X2(I) = X3(I)
TS1(I) = TS2(I)
TS2(I) = TS3(I)
C      CAB1(I) = CAB2(I)
C      CAB2(I) = CAB3(I)
TG1(I) = TG2(I)
TG2(I) = TG3(I)

X3(I) = X(I)
TS3(I) = TS(I)
C      CAB3(I) = CAB(I)
TG3(I) = TG(I)

X(I) = XCT
IF(X(I).GT.XRV(I)) X(I)=1.
TS(I) = TSCT
CAB(I) = CABCT
TG(I) = TGCT

60  CONTINUE

C ----- COMPUTE AT: i = FROM 5 TO INUM

DO 62 I = 5, INUM

CABPD = CAB(I-1)+(DLZ/24.)*(55.*FN1(X(I-1),CAB(I-1))
*      -59.*FN1(X(I-2),CAB(I-2))+37.*FN1(X(I-3),
*      CAB(I-3))-9.*FN1(X(I-4),CAB(I-4)))
IF(ABS(CABPD).LT.EPSI) CABPD= EPSI
TGPD = TG(I-1)+(DLZ/24.)*(55.*FN2(TS(I-1),TG(I-1))
*      -59.*FN2(TS(I-2),TG(I-2))+37.*FN2(TS(I-3),
*      TG(I-3))-9.*FN2(TS(I-4),TG(I-4)))

```

```

XPD = X(I)+(DLT/24.)*(55.*FN3(X(I),CAB(I))
*   -59.*FN3(X3(I),CAB3(I))
*   +37.*FN3(X2(I),CAB2(I))-9.*FN3(X1(I),CAB1(I)))
TSPD = TS(I)+(DLT/24.)*(55.*FN4(TS(I),TG(I),X(I),
*   CAB(I))-59.*FN4(TS3(I),TG3(I),X3(I),CAB3(I))
*   +37.*FN4(TS2(I),TG2(I),X2(I),CAB2(I))
*   -9.*FN4(TS1(I),TG1(I),X1(I),CAB1(I)))
IF(ABS(XPD).LT.EPSI) XPD = EPSI

```

C ----- NUMBER OF CORRECTION

NCRT = 2

DO 666 K = 1,NCRT

```

CABCT = CAB(I-1)+(DLZ/24.)*(9.*FN1(XPD,CABPD)
*   +19.*FN1(X(I-1),CAB(I-1))
*   -5.*FN1(X(I-2),CAB(I-2))+FN1(X(I-3),CAB(I-3)))
IF(ABS(CABCT).LT.EPSI) CABCT = EPSI
TGCT = TG(I-1)+(DLZ/24.)*(9.*FN2(TSPD,TGPD)
*   +19.*FN2(TS(I-1),TG(I-1))
*   -5.*FN2(TS(I-2),TG(I-2))+FN2(TS(I-3),TG(I-3)))
XCT = X(I)+(DLT/24.)*(9.*FN3(XPD,CABCT)+19.*
*   FN3(X(I),CAB(I))-5.*FN3(X3(I),CAB3(I))+
*   FN3(X2(I),CAB2(I)))
IF(ABS(XCT).LT.EPSI) XCT = EPSI
TSCT = TS(I)+(DLT/24.)*(9.*FN4(TSPD,TGCT,XPD,CABCT)
*   +19.*FN4(TS(I),TG(I),X(I),CAB(I))
*   -5.*FN4(TS3(I),TG3(I),X3(I),CAB3(I))
*   +FN4(TS2(I),TG2(I),X2(I),CAB2(I)))

```

CABPD = CABCT

XPD = XCT

TGPD = TGCT

TSPD = TSCT

666 CONTINUE

X1(I) = X2(I)

X2(I) = X3(I)

TS1(I) = TS2(I)

TS2(I) = TS3(I)

C CAB1(I) = CAB2(I)

C CAB2(I) = CAB3(I)

TG1(I) = TG2(I)

TG2(I) = TG3(I)

X3(I) = X(I)

TS3(I) = TS(I)

C CAB3(I) = CAB(I)

TG3(I) = TG(I)

X(I) = XCT

TS(I) = TSCT

CAB(I) = CABCT

```

        TG(I) = TGCT
62    CONTINUE
C ----- GOING TO THE NEXT TIME STEP
        T = T + DLT
C -----
C CHECK THE MAXIMUM SORBENT FRACTIONAL CONVERSION
        DO 70 IINO = 1, INUM
            IF(X(IINO).GT.XRV(IINO)) X(IINO) = 1.
70    CONTINUE
C -----
C NEW5
    IF((.NOT.WTIME).AND.((1.-CAB(INUM))*CABPPM*(2./3.)
    *   .LE.WSO2PM)) THEN

        TIMEW = T
        DO 69 I = 1, INUM
            WRX(I) = X(I)
69    CONTINUE

        WTIME = .TRUE.

    END IF
C -----

    IF((TINT*10.).GE.1.) FACT = 10
    IF((TINT*10.).GE.10.) FACT = 1
    JBGIN = INT(TBGIN*FACT*1.001)
    JINT = INT(TINT*FACT*1.001)
    JEND = INT(TEND*FACT*1.001)

    DO 72 JJ = JBGIN, JEND, JINT

        IF(ABS(T-JJ/FACT).LT.EPS) THEN
            WRITE (6,400) T
        END IF

    DO 77 INO = 1, INUM

        REGTG(I1+INO) = TG(INO)
        REGTS(I1+INO) = TS(INO)
        REGCAB(I1+INO) = CAB(INO)
        REGX(I1+INO) = X(INO)
        XDIF = XRV(INO) - X(INO)
        IF(XDIF.LE.0.) XDIF = 0.
        REGSLD(I1+INO) = FULS*XDIF

```

```

77          CONTINUE

          I1 = I1 + INUM

          PPMEXT(I5) = CAB(INUM)*CABPPM
          PPMO2(I5) = (1.-CAB(INUM))*CABPPM*(2./3.)

          I5 = I5 + 1

          END IF

72          CONTINUE

C ----- FOR TEMP. VS TIME

          DO 81 JT = 1, NTIME

              IF(ABS(T-BTBGIN*JT).LE.EPS) THEN

                  DO 83 NL = 1, NBLIN

                      TGIMSI(NL,NT) = TG(IBPNT(NL))
83              TSIMSI(NL,NT) = TS(IBPNT(NL))

                      NT = NT + 1

                  END IF

81          CONTINUE

C -----

100         CONTINUE

C -----

C NEW 6

          IF(WTIME) THEN

              WRITE(6,101) TIMEW
101          FORMAT(//'TIME FOR WANTED EXIT SO2 PPM = '
                  *,F8.2,'hr')

              DO 103 I = 1, INUM
103          WRITE (15,122) WRX(I)
122          FORMAT (12X,E14.4)

              DO 107 I = 1, INUM
                  XDIF = XRV(I) - WRX(I)
                  IF(XDIF.LE.0) XDIF = 0.
                  WSLOD(I) = FULS*XDIF
107          CONTINUE

              DO 109 I = 1, INUM
109          WRITE(17,133) WSLOD(I)

```

```

133      FORMAT (12X,E14.4)

      ELSE

          WRITE(6,102)
102      FORMAT(//' TIMEW EXCEEDS ENDING TIME !!!')

      END IF

C -----

      NLA = 0

      DO 85 L = 1, NBLIN

          DO 87 M = 1, NT-1

              BTG(NLA+M) = TGIMSI(L,M)
187      BTS(NLA+M) = TSIMSI(L,M)

              NLA = NLA + NT -1

85      CONTINUE

C -----

      NTLIN = INT((TEND-TBGIN)/TINT*1.001) + 1

C ----- SIMULATION RESULTS

      CALL PPMOUT(PPMEXT,PPMSO2,NTLIN,TBGIN,TINT)
      CALL OUTPUT(REGCAB,REGX,REGSLD,REGTG,REGTS,NTLIN,
*              TBGIN,TINT)
      CALL TMPOUT(BBGIN,BINT,NBLIN,BTBGIN,BTG,BTS)

400  FORMAT(// '          INTEGRATED TO ',F9.2,' HR')
      RETURN
      END

C ----- END OF SUBROUTINE AMPC
C *****

C ----- SUBROUTINE PPMOUT

      SUBROUTINE PPMOUT(PPMEXT,PPMSO2,NTLIN,TBGIN,TINT)
      DIMENSION PPMEXT(12550),PPMSO2(12550)
      OPEN(11,FILE='HPM22.DAT',STATUS='NEW')

      WRITE(11,999)
999  FORMAT(/// '          TIME(hr)   EXIT O2(ppm)'
*          '          EXIT SO2(ppm)'//)

      DO 491 I = 2,NTLIN+1
      WRITE(11,888) TBGIN+TINT*(I-2), PPMEXT(I), PPMSO2(I)

```



```

491 CONTINUE

888 FORMAT(10X,F8.2,7X,E10.3,7X,E10.3)

      CLOSE(11)
      RETURN
      END

C ----- SUBROUTINE OUTPUT

      SUBROUTINE OUTPUT(REGCAB,REGX,REGSLD,REGTG,REGTS,
*                       NTLIN,TBGIN,TINT)
      DIMENSION Z(51)
      DIMENSION REGCAB(12550),REGX(12550),REGSLD(12550),
*               REGTG(12550),REGTS(12550)
      COMMON /COM1/ INUM
      OPEN(12,FILE='HP22.DAT',STATUS='NEW')

      I1 = 1

      DO 91 I = 1,51
91      Z(I) = 0. + (I-1)*0.02

      DO 95 I = 1,NTLIN

          WRITE(12,97) TBGIN + TINT*(I-1)

          DO 94 I2 = 1,51
              I3 = I1 + (INUM-1)/50*(I2-1)
94      WRITE(12,98) Z(I2), REGCAB(I3),REGX(I3),REGSLD(I3),
*               REGTG(I3),REGTS(I3)

          I1=I1+INUM

95      CONTINUE

97      FORMAT(//'                               << AT REGENERATION'
* ' TIME ='
* ,F8.3,      ' (hr) >>'
* // '      (Z)      (CAB)      (X)      (SL)'
*           '      (TG)      (TS)'
* /)

98      FORMAT(12X,F5.3,1X,E10.4,1X,E10.4,1X,E10.4,1X,
*             E10.4,1X,E10.4/)

      CLOSE(12)
      RETURN
      END

```

```

C ----- SUBROUTINE TMPOUT

      SUBROUTINE TMPOUT(BBGIN,BINT,NBLIN,BTBGIN,BTG,BTS)
      DIMENSION TIME(51)
      DIMENSION BTG(500), BTS(500)

```

```

COMMON /COM1/ INUM
OPEN(13,FILE='HTP22.DAT',STATUS='NEW')

NTIME = 50
K2 = 0

DO 222 K = 1,NTIME
222   TIME(K) = 0. + K*BTBGIN

DO 223 K1 = 1, NBLIN
WRITE(13,229) BGIN+BINT*(K1-1)

      DO 88 K3 = 1, NTIME
      K2 = K2 + 1
      WRITE(13,77) TIME(K3), BTG(K2),BTS(K2)
88   CONTINUE

223 CONTINUE

229   FORMAT(//'                                << AT BED LOCATION = '
*       ,F8.3,' >>'
*       // '
*           '          TIME          GAS TEMP'
*           '          SORBENT TEMP'
*           /'          (hr)          (TG)'
*           '          (TS)'
*/)
77   FORMAT(11X,F9.4,5X,E11.4,5X,E11.4)

CLOSE(13)
RETURN
END

```

```

C -----
C ----- FUNCTION FN1

FUNCTION FN1(X,CAB)
FN1 = -CAB*BETA(X)
RETURN
END

C ----- FUNCTION FN2

FUNCTION FN2(TS,TG)
COMMON /COM2/ FC2
FN2 = FC2*(TS-TG)
RETURN
END

C ----- FUNCTION FN3

FUNCTION FN3(X,CAB)
COMMON /COM3/ FC1

```

```
FN3 = FC1*BETA(X)*CAB
RETURN
END
```

```
C ----- FUNCTION FN4
```

```
FUNCTION FN4(TS,TG,X,CAB)
COMMON /COM4/ FC3,FC4
FN4 = FC3*RBV(X,CAB)-FC4*(TS-TG)
RETURN
END
```

```
C ----- FUNCTION RBV
```

```
FUNCTION RBV(X,CAB)
COMMON /COM6/ FCRBV
RBV = FCRBV*BETA(X)*CAB
RETURN
END
```

```
C ----- FUNCTION BETA
```

```
FUNCTION BETA(X)
COMMON /COM7/ FCBTA1,FCBTA3,FCBTA2,DE1,R
IF(X.LT.1.) GO TO 201
  BETA = 0.
  RETURN

201 BETA = FCBTA1/(FCBTA2 + (1./((1.-X)**0.5))*FCBTA3
*      -(0.5*R**2/DE1)*LOG(1.-X))

RETURN
END
```

APPENDIX E

OUTPUT FROM REGENERATION SIMULATION

The following are obtained from the regeneration simulation:

- 1) Initial sulfur loading for regeneration,
- 2) Sorbent conversion when exit SO_2 concentration is 1000 ppmv, (Value at each grid point along the regenerator axis is shown.)
- 3) Sulfur loading when exit SO_2 is 1000 ppmv, (Value at each grid point along the regenerator axis is shown.)
- 4) Regeneration time vs exit O_2 and SO_2 concentrations,
- 5) Values of O_2 concentration, sorbent conversion, sulfur loading, gas temperature and sorbent temperature along the regenerator at specified times, and
- 6) Values of gas temperature and sorbent temperature along the time axis at specified bed locations.

Section 1

INITIAL SULFUR LOADING FOR REGENERATION:

Z	SULFUR LOADING
.000	.52872E-03
.020	.32705E-02
.040	.11914E-01
.060	.26029E-01
.080	.42823E-01
.100	.60688E-01
.120	.78882E-01
.140	.96944E-01
.160	.11474E+00
.180	.13212E+00
.200	.14900E+00
.220	.16532E+00
.240	.18105E+00
.260	.19619E+00
.280	.21067E+00
.300	.22449E+00
.320	.23763E+00
.340	.25011E+00
.360	.26190E+00
.380	.27297E+00
.400	.28334E+00
.420	.29293E+00
.440	.30180E+00
.460	.30981E+00
.480	.31694E+00
.500	.32308E+00
.520	.32781E+00
.540	.32840E+00
.560	.32840E+00
.580	.32840E+00
.600	.32840E+00
.620	.32840E+00
.640	.32840E+00
.660	.32840E+00
.680	.32840E+00
.700	.32840E+00
.720	.32840E+00
.740	.32840E+00
.760	.32840E+00
.780	.32840E+00
.800	.32840E+00
.820	.32840E+00
.840	.32840E+00
.860	.32840E+00
.880	.32840E+00

.900	.32840E+00
.920	.32840E+00
.940	.32840E+00
.960	.32840E+00
.980	.32840E+00
1.000	.32840E+00

i=161	.1000E+01	i=184	.1000E+01	i=207	.1000E+01	i=230	.1000E+01
	.1000E+01		.1000E+01		.1000E+01		.1000E+01
	.1000E+01		.1000E+01		.1000E+01		.1000E+01
	.1000E+01		.1000E+01		.1000E+01		.1000E+01
	.1000E+01		.1000E+01		.1000E+01		.1000E+01
	.1000E+01		.1000E+01		.1000E+01		.1000E+01
	.1000E+01		.1000E+01		.1000E+01		.1000E+01
	.1000E+01		.1000E+01		.1000E+01		.1000E+01
	.1000E+01		.1000E+01		.1000E+01		.1000E+01
	.1000E+01		.1000E+01		.1000E+01		.1000E+01
	.1000E+01		.1000E+01		.1000E+01		.9976E+00
	.1000E+01		.1000E+01		.1000E+01		.9946E+00
	.1000E+01		.1000E+01		.1000E+01		.9912E+00
	.1000E+01		.1000E+01		.1000E+01		.9875E+00
	.1000E+01		.1000E+01		.1000E+01		.9836E+00
	.1000E+01		.1000E+01		.1000E+01		.9795E+00
	.1000E+01		.1000E+01		.1000E+01		.9751E+00
	.1000E+01		.1000E+01		.1000E+01		.9705E+00
	.1000E+01		.1000E+01		.1000E+01		.9658E+00
	.1000E+01		.1000E+01		.1000E+01		.9609E+00
	.1000E+01		.1000E+01		.1000E+01		.9558E+00
	.1000E+01		.1000E+01		.1000E+01		.9506E+00
	.1000E+01		.1000E+01		.1000E+01		.9452E+00
	.1000E+01		.1000E+01		.1000E+01		.9396E+00
	.1000E+01		.1000E+01		.1000E+01		.1000E+01

i=161	.0000E+00	i=184	.0000E+00	i=207	.0000E+00	i=230	.0000E+00
	.0000E+00		.0000E+00		.0000E+00		.0000E+00
	.0000E+00		.0000E+00		.0000E+00		.0000E+00
	.0000E+00		.0000E+00		.0000E+00		.0000E+00
	.0000E+00		.0000E+00		.0000E+00		.0000E+00
	.0000E+00		.0000E+00		.0000E+00		.0000E+00
	.0000E+00		.0000E+00		.0000E+00		.0000E+00
	.0000E+00		.0000E+00		.0000E+00		.0000E+00
	.0000E+00		.0000E+00		.0000E+00		.0000E+00
	.0000E+00		.0000E+00		.0000E+00		.7792E-03
	.0000E+00		.0000E+00		.0000E+00		.1773E-02
	.0000E+00		.0000E+00		.0000E+00		.2887E-02
	.0000E+00		.0000E+00		.0000E+00		.4094E-02
	.0000E+00		.0000E+00		.0000E+00		.5384E-02
	.0000E+00		.0000E+00		.0000E+00		.6747E-02
	.0000E+00		.0000E+00		.0000E+00		.8178E-02
	.0000E+00		.0000E+00		.0000E+00		.9672E-02
	.0000E+00		.0000E+00		.0000E+00		.1123E-01
	.0000E+00		.0000E+00		.0000E+00		.1284E-01
	.0000E+00		.0000E+00		.0000E+00		.1451E-01
	.0000E+00		.0000E+00		.0000E+00		.1623E-01
	.0000E+00		.0000E+00		.0000E+00		.1800E-01
	.0000E+00		.0000E+00		.0000E+00		.1982E-01
	.0000E+00		.0000E+00		.0000E+00		.0000E+00

Section 4

TIME(hr)	EXIT O2(ppm)	EXIT SO2(ppm)
.20	.442E-34	.167E+05
.40	.352E-30	.167E+05
.60	.369E-27	.167E+05
.80	.138E-24	.167E+05
1.00	.275E-22	.167E+05
1.20	.350E-20	.167E+05
1.40	.319E-18	.167E+05
1.60	.225E-16	.167E+05
1.80	.130E-14	.167E+05
2.00	.636E-13	.167E+05
2.20	.270E-11	.167E+05
2.40	.101E-09	.167E+05
2.60	.346E-08	.167E+05
2.80	.108E-06	.167E+05
3.00	.311E-05	.167E+05
3.20	.845E-04	.167E+05
3.40	.217E-02	.167E+05
3.60	.536E-01	.167E+05
3.80	.127E+01	.167E+05
4.00	.294E+02	.166E+05
4.20	.449E+03	.164E+05
4.40	.201E+04	.153E+05
4.60	.418E+04	.139E+05
4.80	.649E+04	.123E+05
5.00	.877E+04	.108E+05
5.20	.110E+05	.934E+04
5.40	.131E+05	.794E+04
5.60	.150E+05	.664E+04
5.80	.169E+05	.542E+04
6.00	.185E+05	.430E+04
6.20	.201E+05	.328E+04
6.40	.215E+05	.237E+04
6.60	.227E+05	.156E+04
6.80	.237E+05	.862E+03
7.00	.245E+05	.301E+03
7.20	.250E+05	.000E+00
7.40	.250E+05	.000E+00
7.60	.250E+05	.000E+00
7.80	.250E+05	.000E+00
8.00	.250E+05	.000E+00
8.20	.250E+05	.000E+00
8.40	.250E+05	.000E+00
8.60	.250E+05	.000E+00
8.80	.250E+05	.000E+00
9.00	.250E+05	.000E+00
9.20	.250E+05	.000E+00
9.40	.250E+05	.000E+00
9.60	.250E+05	.000E+00

9.80	.250E+05	.000E+00
10.00	.250E+05	.000E+00

Section 5

<< AT REGENERATION TIME = 1.000 (hr) >>

(Z)	(CAB)	(X)	(SL)	(TG)	(TS)
.000	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.040	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.080	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.120	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.160	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.200	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.240	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.280	.9562E+00	.5858E+00	.1830E-01	.1027E+01	.1059E+01
.320	.7704E+00	.4718E+00	.8268E-01	.1117E+01	.1152E+01
.360	.5691E+00	.3484E+00	.1475E+00	.1216E+01	.1255E+01
.400	.3571E+00	.2185E+00	.2116E+00	.1323E+01	.1364E+01
.440	.1504E+00	.9186E-01	.2716E+00	.1428E+01	.1464E+01
.480	.1568E-01	.9533E-02	.3138E+00	.1493E+01	.1502E+01
.520	.2289E-03	.1389E-03	.3278E+00	.1501E+01	.1501E+01
.560	.2618E-05	.1589E-05	.3284E+00	.1503E+01	.1504E+01
.600	.2983E-07	.1810E-07	.3284E+00	.1505E+01	.1506E+01
.640	.3399E-09	.2062E-09	.3284E+00	.1508E+01	.1509E+01
.680	.3873E-11	.2350E-11	.3284E+00	.1511E+01	.1512E+01
.720	.4413E-13	.2678E-13	.3284E+00	.1515E+01	.1516E+01
.760	.5028E-15	.3051E-15	.3284E+00	.1519E+01	.1521E+01
.800	.5729E-17	.3476E-17	.3284E+00	.1524E+01	.1526E+01
.840	.6527E-19	.3961E-19	.3284E+00	.1530E+01	.1532E+01
.880	.7437E-21	.4513E-21	.3284E+00	.1536E+01	.1538E+01

.920	.8474E-23	.5142E-23	.3284E+00	.1541E+01	.1543E+01
.960	.9655E-25	.5859E-25	.3284E+00	.1545E+01	.1546E+01
1.000	.1100E-26	.6675E-27	.3284E+00	.1545E+01	.1544E+01

<< AT REGENERATION TIME = 2.000 (hr) >>

(Z)	(CAB)	(X)	(SL)	(TG)	(TS)
.000	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.040	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.080	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.120	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.160	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.200	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.240	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.280	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.320	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.360	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.400	.9345E+00	.7703E+00	.3038E-01	.1031E+01	.1049E+01
.440	.8218E+00	.6774E+00	.7936E-01	.1084E+01	.1105E+01
.480	.6952E+00	.5730E+00	.1288E+00	.1144E+01	.1167E+01
.520	.5557E+00	.4579E+00	.1774E+00	.1211E+01	.1237E+01
.560	.4049E+00	.3335E+00	.2189E+00	.1283E+01	.1312E+01
.600	.2469E+00	.2033E+00	.2616E+00	.1360E+01	.1389E+01
.640	.9566E-01	.7866E-01	.3026E+00	.1433E+01	.1458E+01
.680	.7593E-02	.6222E-02	.3264E+00	.1474E+01	.1478E+01
.720	.1018E-03	.8328E-04	.3284E+00	.1477E+01	.1477E+01
.760	.1162E-05	.9510E-06	.3284E+00	.1477E+01	.1478E+01
.800	.1324E-07	.1084E-07	.3284E+00	.1478E+01	.1478E+01

.840	.1509E-09	.1235E-09	.3284E+00	.1478E+01	.1479E+01
.880	.1719E-11	.1407E-11	.3284E+00	.1479E+01	.1479E+01
.920	.1959E-13	.1603E-13	.3284E+00	.1479E+01	.1480E+01
.960	.2232E-15	.1826E-15	.3284E+00	.1480E+01	.1480E+01
1.000	.2543E-17	.2081E-17	.3284E+00	.1481E+01	.1481E+01

<< AT REGENERATION TIME = 3.000 (hr) >>

(Z)	(CAB)	(X)	(SL)	(TG)	(TS)
.000	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.040	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.080	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.120	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.160	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.200	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.240	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.280	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.320	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.360	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.400	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.440	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.480	.9723E+00	.9185E+00	.1530E-01	.1014E+01	.1025E+01
.520	.9000E+00	.8502E+00	.4860E-01	.1047E+01	.1061E+01
.560	.8142E+00	.7691E+00	.7582E-01	.1087E+01	.1103E+01
.600	.7157E+00	.6760E+00	.1064E+00	.1133E+01	.1152E+01
.640	.6051E+00	.5715E+00	.1407E+00	.1185E+01	.1206E+01
.680	.4832E+00	.4563E+00	.1785E+00	.1243E+01	.1265E+01
.720	.3515E+00	.3319E+00	.2194E+00	.1306E+01	.1330E+01

.760	.2137E+00	.2017E+00	.2622E+00	.1371E+01	.1396E+01
.800	.8196E-01	.7726E-01	.3030E+00	.1433E+01	.1454E+01
.840	.6313E-02	.5933E-02	.3265E+00	.1467E+01	.1471E+01
.880	.8399E-04	.7884E-04	.3284E+00	.1470E+01	.1470E+01
.920	.9589E-06	.9001E-06	.3284E+00	.1470E+01	.1470E+01
.960	.1093E-07	.1026E-07	.3284E+00	.1470E+01	.1470E+01
1.000	.1245E-09	.1169E-09	.3284E+00	.1470E+01	.1470E+01

<< AT REGENERATION TIME = 4.000 (hr) >>

(Z)	(CAB)	(X)	(SL)	(TG)	(TS)
.000	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.040	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.080	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.120	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.160	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.200	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.240	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.280	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.320	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.360	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.400	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.440	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.480	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.520	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.560	.9960E+00	.9962E+00	.1260E-02	.1003E+01	.1008E+01
.600	.9531E+00	.9532E+00	.1536E-01	.1023E+01	.1033E+01
.640	.8933E+00	.8934E+00	.3502E-01	.1052E+01	.1064E+01

.680	.8199E+00	.8199E+00	.5913E-01	.1087E+01	.1101E+01
.720	.7341E+00	.7341E+00	.8732E-01	.1128E+01	.1144E+01
.760	.6365E+00	.6365E+00	.1194E+00	.1174E+01	.1193E+01
.800	.5278E+00	.5277E+00	.1551E+00	.1226E+01	.1246E+01
.840	.4088E+00	.4086E+00	.1942E+00	.1282E+01	.1304E+01
.880	.2815E+00	.2813E+00	.2360E+00	.1342E+01	.1365E+01
.920	.1512E+00	.1511E+00	.2788E+00	.1403E+01	.1425E+01
.960	.3849E-01	.3838E-01	.3158E+00	.1455E+01	.1469E+01
1.000	.1177E-02	.1170E-02	.3280E+00	.1470E+01	.1471E+01

<< AT REGENERATION TIME = 5.000 (hr) >>

(Z)	(CAB)	(X)	(SL)	(TG)	(TS)
.000	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.040	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.080	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.120	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.160	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.200	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.240	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.280	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.320	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.360	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.400	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.440	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.480	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.520	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.560	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01

.600	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.640	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.680	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.720	.9784E+00	.9790E+00	.6885E-02	.1011E+01	.1019E+01
.760	.9269E+00	.9275E+00	.2381E-01	.1036E+01	.1046E+01
.800	.8607E+00	.8612E+00	.4558E-01	.1068E+01	.1081E+01
.840	.7816E+00	.7820E+00	.7159E-01	.1105E+01	.1121E+01
.880	.6903E+00	.6907E+00	.1016E+00	.1149E+01	.1166E+01
.920	.5876E+00	.5878E+00	.1354E+00	.1198E+01	.1217E+01
.960	.4740E+00	.4742E+00	.1727E+00	.1252E+01	.1273E+01
1.000	.3509E+00	.3510E+00	.2131E+00	.1311E+01	.1333E+01

<< AT REGENERATION TIME = 6.000 (hr) >>

(Z)	(CAB)	(X)	(SL)	(TG)	(TS)
.000	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.040	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.080	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.120	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.160	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.200	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.240	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.280	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.320	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.360	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.400	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.440	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.480	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01

.520	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.560	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.600	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.640	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.680	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.720	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.760	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.800	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.840	.9990E+00	.9985E+00	.5070E-03	.1001E+01	.1007E+01
.880	.9577E+00	.9574E+00	.1399E-01	.1021E+01	.1031E+01
.920	.8990E+00	.8987E+00	.3326E-01	.1050E+01	.1061E+01
.960	.8267E+00	.8263E+00	.5703E-01	.1084E+01	.1098E+01
1.000	.7418E+00	.7415E+00	.8489E-01	.1125E+01	.1141E+01

<< AT REGENERATION TIME = 7.000 (hr) >>

(Z)	(CAB)	(X)	(SL)	(TG)	(TS)
.000	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.040	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.080	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.120	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.160	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.200	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.240	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.280	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.320	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.360	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.400	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01

.440	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.480	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.520	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.560	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.600	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.640	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.680	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.720	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.760	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.800	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.840	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.880	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.920	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.960	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
1.000	.9820E+00	.9824E+00	.5772E-02	.1009E+01	.1017E+01

<< AT REGENERATION TIME = 8.000 (hr) >>

(Z)	(CAB)	(X)	(SL)	(TG)	(TS)
.000	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.040	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.080	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.120	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.160	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.200	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.240	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.280	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.320	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01

.360	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.400	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.440	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.480	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.520	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.560	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.600	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.640	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.680	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.720	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.760	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.800	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.840	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.880	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.920	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
.960	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01
1.000	.1000E+01	.1000E+01	.0000E+00	.1000E+01	.1000E+01

Section 6

<< AT BED LOCATION = .100 >>

TIME (hr)	GAS TEMP (TG)	SORBENT TEMP (TS)
.2000	.1002E+01	.1004E+01
.4000	.1000E+01	.1000E+01
.6000	.1000E+01	.1000E+01
.8000	.1000E+01	.1000E+01
1.0000	.1000E+01	.1000E+01
1.2000	.1000E+01	.1000E+01
1.4000	.1000E+01	.1000E+01
1.6000	.1000E+01	.1000E+01
1.8000	.1000E+01	.1000E+01
2.0000	.1000E+01	.1000E+01
2.2000	.1000E+01	.1000E+01
2.4000	.1000E+01	.1000E+01
2.6000	.1000E+01	.1000E+01
2.8000	.1000E+01	.1000E+01
3.0000	.1000E+01	.1000E+01
3.2000	.1000E+01	.1000E+01
3.4000	.1000E+01	.1000E+01
3.6000	.1000E+01	.1000E+01
3.8000	.1000E+01	.1000E+01
4.0000	.1000E+01	.1000E+01
4.2000	.1000E+01	.1000E+01
4.4000	.1000E+01	.1000E+01
4.6000	.1000E+01	.1000E+01
4.8000	.1000E+01	.1000E+01
5.0000	.1000E+01	.1000E+01
5.2000	.1000E+01	.1000E+01
5.4000	.1000E+01	.1000E+01
5.6000	.1000E+01	.1000E+01
5.8000	.1000E+01	.1000E+01
6.0000	.1000E+01	.1000E+01
6.2000	.1000E+01	.1000E+01
6.4000	.1000E+01	.1000E+01
6.6000	.1000E+01	.1000E+01
6.8000	.1000E+01	.1000E+01
7.0000	.1000E+01	.1000E+01
7.2000	.1000E+01	.1000E+01
7.4000	.1000E+01	.1000E+01
7.6000	.1000E+01	.1000E+01
7.8000	.1000E+01	.1000E+01
8.0000	.1000E+01	.1000E+01
8.2000	.1000E+01	.1000E+01
8.4000	.1000E+01	.1000E+01
8.6000	.1000E+01	.1000E+01
8.8000	.1000E+01	.1000E+01
9.0000	.1000E+01	.1000E+01

9.2000	.1000E+01	.1000E+01
9.4000	.1000E+01	.1000E+01
9.6000	.1000E+01	.1000E+01
9.8000	.1000E+01	.1000E+01
10.0000	.1000E+01	.1000E+01

<< AT BED LOCATION = .200 >>

TIME (hr)	GAS TEMP (TG)	SORBENT TEMP (TS)
.2000	.1549E+01	.1618E+01
.4000	.1106E+01	.1171E+01
.6000	.1000E+01	.1000E+01
.8000	.1000E+01	.1000E+01
1.0000	.1000E+01	.1000E+01
1.2000	.1000E+01	.1000E+01
1.4000	.1000E+01	.1000E+01
1.6000	.1000E+01	.1000E+01
1.8000	.1000E+01	.1000E+01
2.0000	.1000E+01	.1000E+01
2.2000	.1000E+01	.1000E+01
2.4000	.1000E+01	.1000E+01
2.6000	.1000E+01	.1000E+01
2.8000	.1000E+01	.1000E+01
3.0000	.1000E+01	.1000E+01
3.2000	.1000E+01	.1000E+01
3.4000	.1000E+01	.1000E+01
3.6000	.1000E+01	.1000E+01
3.8000	.1000E+01	.1000E+01
4.0000	.1000E+01	.1000E+01
4.2000	.1000E+01	.1000E+01
4.4000	.1000E+01	.1000E+01
4.6000	.1000E+01	.1000E+01
4.8000	.1000E+01	.1000E+01
5.0000	.1000E+01	.1000E+01
5.2000	.1000E+01	.1000E+01
5.4000	.1000E+01	.1000E+01
5.6000	.1000E+01	.1000E+01
5.8000	.1000E+01	.1000E+01
6.0000	.1000E+01	.1000E+01
6.2000	.1000E+01	.1000E+01
6.4000	.1000E+01	.1000E+01
6.6000	.1000E+01	.1000E+01
6.8000	.1000E+01	.1000E+01
7.0000	.1000E+01	.1000E+01
7.2000	.1000E+01	.1000E+01
7.4000	.1000E+01	.1000E+01
7.6000	.1000E+01	.1000E+01
7.8000	.1000E+01	.1000E+01
8.0000	.1000E+01	.1000E+01
8.2000	.1000E+01	.1000E+01
8.4000	.1000E+01	.1000E+01

8.6000	.1000E+01	.1000E+01
8.8000	.1000E+01	.1000E+01
9.0000	.1000E+01	.1000E+01
9.2000	.1000E+01	.1000E+01
9.4000	.1000E+01	.1000E+01
9.6000	.1000E+01	.1000E+01
9.8000	.1000E+01	.1000E+01
10.0000	.1000E+01	.1000E+01

<< AT BED LOCATION = .300 >>

TIME (hr)	GAS TEMP (TG)	SORBENT TEMP (TS)
.2000	.1375E+01	.1319E+01
.4000	.1547E+01	.1584E+01
.6000	.1301E+01	.1356E+01
.8000	.1157E+01	.1199E+01
1.0000	.1071E+01	.1104E+01
1.2000	.1016E+01	.1043E+01
1.4000	.1000E+01	.1000E+01
1.6000	.1000E+01	.1000E+01
1.8000	.1000E+01	.1000E+01
2.0000	.1000E+01	.1000E+01
2.2000	.1000E+01	.1000E+01
2.4000	.1000E+01	.1000E+01
2.6000	.1000E+01	.1000E+01
2.8000	.1000E+01	.1000E+01
3.0000	.1000E+01	.1000E+01
3.2000	.1000E+01	.1000E+01
3.4000	.1000E+01	.1000E+01
3.6000	.1000E+01	.1000E+01
3.8000	.1000E+01	.1000E+01
4.0000	.1000E+01	.1000E+01
4.2000	.1000E+01	.1000E+01
4.4000	.1000E+01	.1000E+01
4.6000	.1000E+01	.1000E+01
4.8000	.1000E+01	.1000E+01
5.0000	.1000E+01	.1000E+01
5.2000	.1000E+01	.1000E+01
5.4000	.1000E+01	.1000E+01
5.6000	.1000E+01	.1000E+01
5.8000	.1000E+01	.1000E+01
6.0000	.1000E+01	.1000E+01
6.2000	.1000E+01	.1000E+01
6.4000	.1000E+01	.1000E+01
6.6000	.1000E+01	.1000E+01
6.8000	.1000E+01	.1000E+01
7.0000	.1000E+01	.1000E+01
7.2000	.1000E+01	.1000E+01
7.4000	.1000E+01	.1000E+01
7.6000	.1000E+01	.1000E+01
7.8000	.1000E+01	.1000E+01

8.0000	.1000E+01	.1000E+01
8.2000	.1000E+01	.1000E+01
8.4000	.1000E+01	.1000E+01
8.6000	.1000E+01	.1000E+01
8.8000	.1000E+01	.1000E+01
9.0000	.1000E+01	.1000E+01
9.2000	.1000E+01	.1000E+01
9.4000	.1000E+01	.1000E+01
9.6000	.1000E+01	.1000E+01
9.8000	.1000E+01	.1000E+01
10.0000	.1000E+01	.1000E+01

<< AT BED LOCATION = .400 >>

TIME (hr)	GAS TEMP (TG)	SORBENT TEMP (TS)
.2000	.1095E+01	.1071E+01
.4000	.1592E+01	.1586E+01
.6000	.1534E+01	.1538E+01
.8000	.1451E+01	.1488E+01
1.0000	.1323E+01	.1364E+01
1.2000	.1225E+01	.1260E+01
1.4000	.1154E+01	.1184E+01
1.6000	.1101E+01	.1126E+01
1.8000	.1061E+01	.1083E+01
2.0000	.1031E+01	.1049E+01
2.2000	.1008E+01	.1024E+01
2.4000	.1000E+01	.1000E+01
2.6000	.1000E+01	.1000E+01
2.8000	.1000E+01	.1000E+01
3.0000	.1000E+01	.1000E+01
3.2000	.1000E+01	.1000E+01
3.4000	.1000E+01	.1000E+01
3.6000	.1000E+01	.1000E+01
3.8000	.1000E+01	.1000E+01
4.0000	.1000E+01	.1000E+01
4.2000	.1000E+01	.1000E+01
4.4000	.1000E+01	.1000E+01
4.6000	.1000E+01	.1000E+01
4.8000	.1000E+01	.1000E+01
5.0000	.1000E+01	.1000E+01
5.2000	.1000E+01	.1000E+01
5.4000	.1000E+01	.1000E+01
5.6000	.1000E+01	.1000E+01
5.8000	.1000E+01	.1000E+01
6.0000	.1000E+01	.1000E+01
6.2000	.1000E+01	.1000E+01
6.4000	.1000E+01	.1000E+01
6.6000	.1000E+01	.1000E+01
6.8000	.1000E+01	.1000E+01
7.0000	.1000E+01	.1000E+01
7.2000	.1000E+01	.1000E+01

7.4000	.1000E+01	.1000E+01
7.6000	.1000E+01	.1000E+01
7.8000	.1000E+01	.1000E+01
8.0000	.1000E+01	.1000E+01
8.2000	.1000E+01	.1000E+01
8.4000	.1000E+01	.1000E+01
8.6000	.1000E+01	.1000E+01
8.8000	.1000E+01	.1000E+01
9.0000	.1000E+01	.1000E+01
9.2000	.1000E+01	.1000E+01
9.4000	.1000E+01	.1000E+01
9.6000	.1000E+01	.1000E+01
9.8000	.1000E+01	.1000E+01
10.0000	.1000E+01	.1000E+01

<< AT BED LOCATION = .500 >>

TIME (hr)	GAS TEMP (TG)	SORBENT TEMP (TS)
.2000	.1013E+01	.1009E+01
.4000	.1463E+01	.1432E+01
.6000	.1560E+01	.1563E+01
.8000	.1516E+01	.1518E+01
1.0000	.1499E+01	.1501E+01
1.2000	.1458E+01	.1484E+01
1.4000	.1372E+01	.1406E+01
1.6000	.1293E+01	.1325E+01
1.8000	.1229E+01	.1257E+01
2.0000	.1176E+01	.1201E+01
2.2000	.1134E+01	.1156E+01
2.4000	.1099E+01	.1119E+01
2.6000	.1071E+01	.1088E+01
2.8000	.1048E+01	.1063E+01
3.0000	.1030E+01	.1042E+01
3.2000	.1015E+01	.1025E+01
3.4000	.1004E+01	.1012E+01
3.6000	.1000E+01	.1000E+01
3.8000	.1000E+01	.1000E+01
4.0000	.1000E+01	.1000E+01
4.2000	.1000E+01	.1000E+01
4.4000	.1000E+01	.1000E+01
4.6000	.1000E+01	.1000E+01
4.8000	.1000E+01	.1000E+01
5.0000	.1000E+01	.1000E+01
5.2000	.1000E+01	.1000E+01
5.4000	.1000E+01	.1000E+01
5.6000	.1000E+01	.1000E+01
5.8000	.1000E+01	.1000E+01
6.0000	.1000E+01	.1000E+01
6.2000	.1000E+01	.1000E+01
6.4000	.1000E+01	.1000E+01
6.6000	.1000E+01	.1000E+01

6.8000	.1000E+01	.1000E+01
7.0000	.1000E+01	.1000E+01
7.2000	.1000E+01	.1000E+01
7.4000	.1000E+01	.1000E+01
7.6000	.1000E+01	.1000E+01
7.8000	.1000E+01	.1000E+01
8.0000	.1000E+01	.1000E+01
8.2000	.1000E+01	.1000E+01
8.4000	.1000E+01	.1000E+01
8.6000	.1000E+01	.1000E+01
8.8000	.1000E+01	.1000E+01
9.0000	.1000E+01	.1000E+01
9.2000	.1000E+01	.1000E+01
9.4000	.1000E+01	.1000E+01
9.6000	.1000E+01	.1000E+01
9.8000	.1000E+01	.1000E+01
10.0000	.1000E+01	.1000E+01

<< AT BED LOCATION = .600 >>

TIME (hr)	GAS TEMP (TG)	SORBENT TEMP (TS)
.2000	.1001E+01	.1001E+01
.4000	.1239E+01	.1208E+01
.6000	.1568E+01	.1564E+01
.8000	.1529E+01	.1532E+01
1.0000	.1505E+01	.1506E+01
1.2000	.1494E+01	.1494E+01
1.4000	.1487E+01	.1487E+01
1.6000	.1475E+01	.1484E+01
1.8000	.1425E+01	.1452E+01
2.0000	.1360E+01	.1389E+01
2.2000	.1300E+01	.1328E+01
2.4000	.1248E+01	.1273E+01
2.6000	.1204E+01	.1227E+01
2.8000	.1166E+01	.1186E+01
3.0000	.1133E+01	.1152E+01
3.2000	.1105E+01	.1121E+01
3.4000	.1081E+01	.1095E+01
3.6000	.1060E+01	.1073E+01
3.8000	.1042E+01	.1053E+01
4.0000	.1023E+01	.1033E+01
4.2000	.1008E+01	.1015E+01
4.4000	.1000E+01	.1000E+01
4.6000	.1000E+01	.1000E+01
4.8000	.1000E+01	.1000E+01
5.0000	.1000E+01	.1000E+01
5.2000	.1000E+01	.1000E+01
5.4000	.1000E+01	.1000E+01
5.6000	.1000E+01	.1000E+01
5.8000	.1000E+01	.1000E+01
6.0000	.1000E+01	.1000E+01

6.2000	.1000E+01	.1000E+01
6.4000	.1000E+01	.1000E+01
6.6000	.1000E+01	.1000E+01
6.8000	.1000E+01	.1000E+01
7.0000	.1000E+01	.1000E+01
7.2000	.1000E+01	.1000E+01
7.4000	.1000E+01	.1000E+01
7.6000	.1000E+01	.1000E+01
7.8000	.1000E+01	.1000E+01
8.0000	.1000E+01	.1000E+01
8.2000	.1000E+01	.1000E+01
8.4000	.1000E+01	.1000E+01
8.6000	.1000E+01	.1000E+01
8.8000	.1000E+01	.1000E+01
9.0000	.1000E+01	.1000E+01
9.2000	.1000E+01	.1000E+01
9.4000	.1000E+01	.1000E+01
9.6000	.1000E+01	.1000E+01
9.8000	.1000E+01	.1000E+01
10.0000	.1000E+01	.1000E+01

<< AT BED LOCATION = .700 >>

TIME (hr)	GAS TEMP (TG)	SORBENT TEMP (TS)
.2000	.1000E+01	.1000E+01
.4000	.1082E+01	.1066E+01
.6000	.1495E+01	.1476E+01
.8000	.1548E+01	.1550E+01
1.0000	.1513E+01	.1514E+01
1.2000	.1498E+01	.1499E+01
1.4000	.1489E+01	.1490E+01
1.6000	.1484E+01	.1484E+01
1.8000	.1480E+01	.1480E+01
2.0000	.1476E+01	.1477E+01
2.2000	.1465E+01	.1476E+01
2.4000	.1423E+01	.1447E+01
2.6000	.1370E+01	.1396E+01
2.8000	.1319E+01	.1344E+01
3.0000	.1274E+01	.1297E+01
3.2000	.1233E+01	.1254E+01
3.4000	.1196E+01	.1216E+01
3.6000	.1164E+01	.1182E+01
3.8000	.1135E+01	.1151E+01
4.0000	.1107E+01	.1122E+01
4.2000	.1079E+01	.1093E+01
4.4000	.1055E+01	.1067E+01
4.6000	.1033E+01	.1044E+01
4.8000	.1015E+01	.1024E+01
5.0000	.1002E+01	.1007E+01
5.2000	.1000E+01	.1000E+01
5.4000	.1000E+01	.1000E+01

5.6000	.1000E+01	.1000E+01
5.8000	.1000E+01	.1000E+01
6.0000	.1000E+01	.1000E+01
6.2000	.1000E+01	.1000E+01
6.4000	.1000E+01	.1000E+01
6.6000	.1000E+01	.1000E+01
6.8000	.1000E+01	.1000E+01
7.0000	.1000E+01	.1000E+01
7.2000	.1000E+01	.1000E+01
7.4000	.1000E+01	.1000E+01
7.6000	.1000E+01	.1000E+01
7.8000	.1000E+01	.1000E+01
8.0000	.1000E+01	.1000E+01
8.2000	.1000E+01	.1000E+01
8.4000	.1000E+01	.1000E+01
8.6000	.1000E+01	.1000E+01
8.8000	.1000E+01	.1000E+01
9.0000	.1000E+01	.1000E+01
9.2000	.1000E+01	.1000E+01
9.4000	.1000E+01	.1000E+01
9.6000	.1000E+01	.1000E+01
9.8000	.1000E+01	.1000E+01
10.0000	.1000E+01	.1000E+01

<< AT BED LOCATION = .800 >>

TIME (hr)	GAS TEMP (TG)	SORBENT TEMP (TS)
.2000	.1000E+01	.1000E+01
.4000	.1019E+01	.1015E+01
.6000	.1335E+01	.1308E+01
.8000	.1554E+01	.1552E+01
1.0000	.1524E+01	.1526E+01
1.2000	.1503E+01	.1504E+01
1.4000	.1492E+01	.1493E+01
1.6000	.1486E+01	.1486E+01
1.8000	.1481E+01	.1481E+01
2.0000	.1478E+01	.1478E+01
2.2000	.1475E+01	.1475E+01
2.4000	.1473E+01	.1473E+01
2.6000	.1471E+01	.1472E+01
2.8000	.1464E+01	.1472E+01
3.0000	.1433E+01	.1454E+01
3.2000	.1389E+01	.1413E+01
3.4000	.1344E+01	.1368E+01
3.6000	.1301E+01	.1324E+01
3.8000	.1262E+01	.1283E+01
4.0000	.1226E+01	.1246E+01
4.2000	.1189E+01	.1208E+01
4.4000	.1155E+01	.1172E+01
4.6000	.1123E+01	.1139E+01
4.8000	.1094E+01	.1108E+01

5.0000	.1068E+01	.1081E+01
5.2000	.1044E+01	.1056E+01
5.4000	.1025E+01	.1034E+01
5.6000	.1008E+01	.1016E+01
5.8000	.1000E+01	.1000E+01
6.0000	.1000E+01	.1000E+01
6.2000	.1000E+01	.1000E+01
6.4000	.1000E+01	.1000E+01
6.6000	.1000E+01	.1000E+01
6.8000	.1000E+01	.1000E+01
7.0000	.1000E+01	.1000E+01
7.2000	.1000E+01	.1000E+01
7.4000	.1000E+01	.1000E+01
7.6000	.1000E+01	.1000E+01
7.8000	.1000E+01	.1000E+01
8.0000	.1000E+01	.1000E+01
8.2000	.1000E+01	.1000E+01
8.4000	.1000E+01	.1000E+01
8.6000	.1000E+01	.1000E+01
8.8000	.1000E+01	.1000E+01
9.0000	.1000E+01	.1000E+01
9.2000	.1000E+01	.1000E+01
9.4000	.1000E+01	.1000E+01
9.6000	.1000E+01	.1000E+01
9.8000	.1000E+01	.1000E+01
10.0000	.1000E+01	.1000E+01

<< AT BED LOCATION = .900 >>

TIME (hr)	GAS TEMP (TG)	SORBENT TEMP (TS)
.2000	.1000E+01	.1000E+01
.4000	.1003E+01	.1002E+01
.6000	.1170E+01	.1150E+01
.8000	.1509E+01	.1497E+01
1.0000	.1539E+01	.1541E+01
1.2000	.1510E+01	.1511E+01
1.4000	.1496E+01	.1497E+01
1.6000	.1488E+01	.1489E+01
1.8000	.1483E+01	.1483E+01
2.0000	.1479E+01	.1479E+01
2.2000	.1476E+01	.1476E+01
2.4000	.1474E+01	.1474E+01
2.6000	.1472E+01	.1472E+01
2.8000	.1471E+01	.1471E+01
3.0000	.1470E+01	.1470E+01
3.2000	.1469E+01	.1469E+01
3.4000	.1467E+01	.1470E+01
3.6000	.1449E+01	.1465E+01
3.8000	.1413E+01	.1434E+01
4.0000	.1373E+01	.1396E+01
4.2000	.1331E+01	.1354E+01

4.4000	.1288E+01	.1310E+01
4.6000	.1248E+01	.1268E+01
4.8000	.1209E+01	.1229E+01
5.0000	.1173E+01	.1191E+01
5.2000	.1139E+01	.1156E+01
5.4000	.1109E+01	.1124E+01
5.6000	.1081E+01	.1095E+01
5.8000	.1056E+01	.1069E+01
6.0000	.1035E+01	.1045E+01
6.2000	.1016E+01	.1025E+01
6.4000	.1003E+01	.1008E+01
6.6000	.1000E+01	.1000E+01
6.8000	.1000E+01	.1000E+01
7.0000	.1000E+01	.1000E+01
7.2000	.1000E+01	.1000E+01
7.4000	.1000E+01	.1000E+01
7.6000	.1000E+01	.1000E+01
7.8000	.1000E+01	.1000E+01
8.0000	.1000E+01	.1000E+01
8.2000	.1000E+01	.1000E+01
8.4000	.1000E+01	.1000E+01
8.6000	.1000E+01	.1000E+01
8.8000	.1000E+01	.1000E+01
9.0000	.1000E+01	.1000E+01
9.2000	.1000E+01	.1000E+01
9.4000	.1000E+01	.1000E+01
9.6000	.1000E+01	.1000E+01
9.8000	.1000E+01	.1000E+01
10.0000	.1000E+01	.1000E+01

<< AT BED LOCATION = 1.000 >>

TIME (hr)	GAS TEMP (TG)	SORBENT TEMP (TS)
.2000	.1000E+01	.1000E+01
.4000	.1000E+01	.1000E+01
.6000	.1065E+01	.1055E+01
.8000	.1396E+01	.1375E+01
1.0000	.1545E+01	.1544E+01
1.2000	.1520E+01	.1522E+01
1.4000	.1501E+01	.1502E+01
1.6000	.1491E+01	.1492E+01
1.8000	.1485E+01	.1485E+01
2.0000	.1481E+01	.1481E+01
2.2000	.1477E+01	.1478E+01
2.4000	.1475E+01	.1475E+01
2.6000	.1473E+01	.1473E+01
2.8000	.1472E+01	.1472E+01
3.0000	.1470E+01	.1470E+01
3.2000	.1470E+01	.1470E+01
3.4000	.1469E+01	.1469E+01
3.6000	.1469E+01	.1469E+01

3.8000	.1469E+01	.1469E+01
4.0000	.1470E+01	.1471E+01
4.2000	.1466E+01	.1475E+01
4.4000	.1439E+01	.1458E+01
4.6000	.1398E+01	.1421E+01
4.8000	.1354E+01	.1378E+01
5.0000	.1311E+01	.1333E+01
5.2000	.1269E+01	.1291E+01
5.4000	.1229E+01	.1249E+01
5.6000	.1192E+01	.1211E+01
5.8000	.1157E+01	.1175E+01
6.0000	.1125E+01	.1141E+01
6.2000	.1095E+01	.1110E+01
6.4000	.1069E+01	.1082E+01
6.6000	.1046E+01	.1057E+01
6.8000	.1026E+01	.1035E+01
7.0000	.1009E+01	.1017E+01
7.2000	.1000E+01	.1000E+01
7.4000	.1000E+01	.1000E+01
7.6000	.1000E+01	.1000E+01
7.8000	.1000E+01	.1000E+01
8.0000	.1000E+01	.1000E+01
8.2000	.1000E+01	.1000E+01
8.4000	.1000E+01	.1000E+01
8.6000	.1000E+01	.1000E+01
8.8000	.1000E+01	.1000E+01
9.0000	.1000E+01	.1000E+01
9.2000	.1000E+01	.1000E+01
9.4000	.1000E+01	.1000E+01
9.6000	.1000E+01	.1000E+01
9.8000	.1000E+01	.1000E+01
10.0000	.1000E+01	.1000E+01

VITA

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