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A Study of Selected Phenomena Observed During Rotary Kiln Incineration.

Christopher Brian Leger

Louisiana State University and Agricultural & Mechanical College

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A study of selected phenomena observed during rotary kiln incineration

Leger, Christopher Brian, Ph.D.

The Louisiana State University and Agricultural and Mechanical Col., 1992
A STUDY OF SELECTED PHENOMENA OBSERVED DURING ROTARY KILN INCINERATION

A Dissertation

Submitted to the Graduate Faculty of the Louisiana State University and Agricultural and Mechanical College in partial fulfillment of the requirements for the degree of Doctor of Philosophy

in

The Department of Mechanical Engineering

by

Christopher Brian Leger
B.S. in M.E., Louisiana State University, 1987
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ABSTRACT

A comprehensive research program is underway at LSU with the ultimate goal of improved understanding and predictive capability for the performance of rotary kiln incinerators.

In an extensive experimental study, packs containing toluene-contaminated clay sorbent are batch-fed into the field-scale rotary kiln incinerator of the Louisiana Division of Dow Chemical USA. Water cooled probes are used to obtain continuously gas temperatures and species concentrations within the kiln and afterburner, and existing facility instruments are also monitored. The kiln rotation rate is varied and turbulence air (air injected into the kiln to improve mixing) is added or turned off. Conditions at the kiln exit are found to be highly stratified. Species data from the afterburner and stack are used to determine the toluene evolution rate, which appears to be strongly influenced by bed motion regime but not kiln rotation rate or turbulence air. Mass balances are performed on the toluene, with good results.

A numerical model of the Dow rotary kiln incinerator is formulated to predict the species, temperature, and flow field during baseline operation with no waste combustion. This simplified model shows the general features and trends at locations where experimental measurements are not feasible. The model is used in a parametric study to determine the influence of turbulence air addition and the importance of buoyancy. The model is developed using the commercially available finite difference software, FLUENT, and solved on a 486 PC computer. The numerical results agree surprisingly well with the experimental data, offering a clearer picture of the buoyant flow field in the kiln.
A pilot-scale rotary kiln simulator at The University of Utah is used to make experimental measurements of the thermal response of solids charged onto a preexisting bed of hot solids. Time constants for solids mixing are extracted from the measurements, and a simple model is developed that correlates the mixing time constant to bed turnover rate. The use of this correlation is then demonstrated in predicting the thermal history of a fresh charge of solids as it mixes with hot solids in a rotary kiln.
CHAPTER 1

INTRODUCTION AND BACKGROUND

DEFINITION AND THE FOUR LAWS OF HAZARDOUS WASTE

There are currently two commonly used definitions for hazardous waste. The first definition is broad and can be broken down into two parts. Hazardous refers to anything toxic or dangerous to the environment or to humans. Waste is defined as anything that is considered worthless or nearly so, such that the owner or producer wants to discard it. Under this broad definition, everything from sewage to broken glass to spoiled food can be considered hazardous waste.

The more specific definition in common use today is that hazardous waste consists of toxic or environmentally harmful chemicals, or materials contaminated with such chemicals, which the owner or producer would like to discard. Usually these chemicals are worthless byproducts of profitable chemical processes, or they may be mixtures of chemicals that would be of value if they were not mixed together. Metal contaminated sludges, used solvents, old pesticides, and soil contaminated with various chemicals are examples that fit this definition of hazardous waste.

How does one clarify the problem of dealing with hazardous waste? A very interesting approach is taken by Thibodeaux (1990), in which he describes four natural laws that apply to hazardous waste. He defines a natural law as "absolute, not subject to repeal by humans." His first law of hazardous waste is: "I am therefore I pollute." This embodies the fact that human beings, because we consume food for sustenance, produce
waste. Humans also engage in constructive activities in which they manipulate their environment and produce desirable goods or effects. All of these activities produce waste in one form or another. Building a fire produces ashes, eating a banana leaves a banana peel, even breathing releases \( \text{CO}_2 \). A corollary to the first law is: "... all manufactured products also generate waste." Since we live in a highly industrialized world, our potential for generating waste in this fashion is tremendous.

The second law of hazardous waste is: "... complete waste recycling is impossible." This follows directly from the first law. Since recycling requires manufacturing something of value from the waste, it will produce some waste in the process. Recycling can reduce the net amount of waste produced, but it cannot totally eliminate waste.

The third law of hazardous waste involves disposal. Since waste is by definition something that the owner or producer would like to discard, the ultimate fate of all waste is disposal in some fashion. The third law states: "the proper disposal of a hazardous waste entails conversion of offensive substances to environmentally compatible materials." The environmental compatibility of the materials is not something that is easily gauged, because the natural environment sets this standard. However, the effects of these end materials on the environment can be studied carefully to determine how "proper" a particular disposal method is.

The fourth law of hazardous waste is: "... small waste leaks [or releases] are unavoidable and acceptable. Ecosystems can safely handle small leaks of hazardous substances." Nature has always handled naturally occurring hazardous substances, many of which are chemically identical to those produced by human processes. This is fortunate because the third law says that proper disposal entails conversion to environmentally compatible materials, while the first law holds that this cannot be accomplished with 100% efficiency. The overriding question to be addressed is: for any given hazardous material, how small a release into the environment is small enough?
The job of determining what quantities of hazardous waste can be released safely into the environment will require much effort from people with many different disciplines. A mechanical engineer's background is not well suited for this type of research. However, it is suitable for addressing a question involving the third law: how can conversion of offensive substances to environmentally compatible materials be achieved in a manner that is cost effective and releases only acceptably small quantities of hazardous substances to the environment? This is the general question with which this study is concerned.

There are many methods for treating, converting, or destroying various types of hazardous waste. One method commonly used is to burn the waste, and this is often accomplished in a rotary kiln incinerator. The scope of this study will be limited to rotary kiln incinerators. The ultimate question to be answered about rotary kiln incinerators is: how can the process be designed or optimized to improve cost effectiveness and performance? To improve or optimize the next generation of rotary kilns, one must be able to predict their performance and determine how improvements can be made. For this, a model that can accurately characterize the system is needed. In order to develop such a model, one must answer the final question: What are the processes occurring within a rotary kiln incinerator, and how do they impact the overall performance? Once the details of the overall process are understood, a predictive model may be developed which can facilitate design and optimization of the process.

DESCRIPTION OF A ROTARY KILN INCINERATOR

A rotary kiln is a refractory-lined, cylindrical shell through which fuel, air, and solid process materials flow. The cylinder is typically mounted horizontally on rollers that allow the kiln to rotate, and it usually has a slight incline to facilitate the flow of solids (see Figure 1.1). In a rotary kiln incinerator, the objective is to vaporize and combust any volatile organic chemicals in the waste. The result is a reduction in solids volume and
the destruction of the hazardous organic components. Most rotary kiln incinerators are capable of handling many types of solid, liquid, and gaseous wastes. This is why they are so versatile in handling a variety of waste streams, in contrast to many other types of incinerators that only handle homogeneous waste streams. The rotary kiln incinerators of today have evolved from rotary lime kiln and rotary cement kiln technology, where the processing of large quantities of solids at high temperatures was the objective.

Figure 1.1 Schematic diagram of a typical rotary kiln incinerator facility.

In a typical rotary kiln incinerator, waste enters the kiln on the elevated end. Bulk solids may be fed via conveyor belt, gravity chute, screw-feeder, or hydraulic ram. Often, drummed waste is fed directly, barrel included, with a gravity chute or hydraulic ram. Liquid wastes are often introduced into the kiln using atomizing nozzles. High heating value waste may be fed through specially modified burners where it is mixed with air and combusted. Sludges and slurries with high water or high solids content are often piped directly into the kiln where the liquids vaporize and the solids remain.
Once inside the kiln, the waste undergoes a variety of processes (see Figure 1.2). Solids fall to the kiln floor where they are heated by convection from the gas, conduction from the wall, radiation from the support flame, and mixing with hot solids. Rotation of the kiln facilitates mixing of the solids and forms a bed of loose solid material that progresses toward the kiln exit. Volatile species present in the solids are driven off by the heating. These volatiles, along with liquids atomized into the kiln, enter the gas phase where they combust or decompose. The combustion of these volatile species often provides a large fraction of the heat needed to sustain the process. However, depending upon the heating value of the waste, auxiliary fuel may be introduced into the system through a support burner. Typically, the kiln is operated at temperatures between 800° C and 1700° C, with gas phase residence times greater than 2 seconds and solid phase residence times between 15 minutes and 2 hours.

Figure 1.2 Processes involved in rotary kiln incineration of containerized waste.
A typical process flow diagram for a rotary kiln incinerator facility was shown in Figure 1.1. This drawing shows a co-current design in which the gas and solid streams flow in the same direction through the kiln. Counter-current designs, in which the gas and solid streams flow in opposite directions, are also common. In the co-current design, waste, fuel, and combustion air are fed into one end of the kiln for processing. Hot ash exits the other end of the kiln, where it falls into a hopper car or a water quench basin. Most rotary kiln incinerator ash is then landfilled. The hot combustion gas from the kiln typically contains acid gases, particulates, and sometimes hazardous chemical species that have not been fully destroyed. This gas enters the afterburner where additional fuel and air are introduced, and the temperature is raised to destroy any remaining hazardous species. The hot gas then may pass through a heat recovery boiler, however this piece of equipment is often not cost effective because of the highly corrosive nature of the gas stream. The hot gas typically undergoes a quench stage where water is sprayed into the gas to cool it before it enters the other pollution control equipment. This is often accomplished with a venturi scrubber, which also serves to remove some acid gases and some particulates from the stream. This quenched gas flows into acid gas removal equipment, usually consisting of a packed column or a spray tower, where a caustic solution is contacted with the gas to neutralize the acid. Then the stream passes into particulate control equipment, such as electrostatic precipitators or baghouses, where the fly ash and caustic particulates are removed. Finally, the gas flows through the induced draft fan and up the stack.

The induced draft fan provides the motive force for gas flow through the system. Rotary kiln incinerators use induced draft flow because it causes the system to operate at a slight vacuum so that any small leaks in the system allow air to leak in and no waste can escape. Air leaks are normally present in rotary kiln incinerators because of the rotary nature of the equipment. The rotating kiln must be connected to the fixed feed and exhaust equipment through high temperature rotary seals, which typically allow
substantial amounts of air to leak into the kiln. The amount of this leakage can be controlled somewhat by varying the kiln pressure, and this is often one of the methods used to introduce additional combustion air to the system.

In some rotary kiln incinerators, part of the secondary air for combustion of the waste is provided through nozzles near the support burners. Because the nozzles inject compressed air into the system, high velocities are produced which tend to induce turbulence and bulk mixing within the kiln. This nozzle supplied secondary air is typically referred to as “turbulence air”.

In rotary kiln incinerators which process solids, the layer of solids on the floor of the kiln is called the bed. This layer may be anywhere from a few centimeters thick up to a few meters. The degree to which solids fill the kiln is called the fill fraction, and it is defined as the ratio of the volume of solids in the kiln to the total volume of the kiln. The fill fraction may vary along the axis of the kiln, and in such cases the fill fraction is defined as the ratio of the axial cross sectional area of bed to the axial cross sectional area of the kiln at a particular axial location. In hazardous waste incinerators, fill fractions of less than 20% are common, although trace contaminated soils may be processed at much higher fill fractions. The solids bed in most systems consists of ash, metal fragments, soil, or sorbent material that was intentionally used to pick up spilled waste.

The primary advantages of the rotary kiln incinerator are all related to its flexibility in handling diverse waste streams. Rotary kilns can handle solid material of very non-homogeneous size characteristics, including very fine materials and large, bulky items such as barrels and boxes. They can also handle liquid and sludge streams simultaneously. The ability to destroy containerized waste without having to remove it from the container is a big advantage. The mixing of the solids caused by the rotating motion of the kiln results in heating of the solid material and volatilization of the waste, even for large, bulky items. The use of a support flame allows the system to process large quantities of slightly combustible wastes, such as contaminated soils.
According to Theodore and Reynolds (1987), disadvantages of the rotary kiln incinerator include: high capital and operating costs; the need for highly trained personnel required to operate the complicated facility; frequent replacement of the refractory lining if the waste stream is very abrasive or corrosive; and the generation of fine particulates due to the cascading action of the solids in the kiln. One difficulty peculiar to rotary kiln incinerators is the possibility of fugitive waste emissions during positive pressure excursions. The introduction of containerized waste into a rotary kiln incinerator results in transient behavior as the large amount of volatile material from each container is combusted. Sometimes very rapid combustion occurs, resulting in a rapid pressure rise in the kiln and the possibility of unburned waste leaking out through the rotary seals. These excursions from baseline operation are commonly called "puffs" (Linak et al. 1987a), and are generally controlled by limiting the amount of volatiles introduced in any one container and by operating at an average waste feed rate that is well below the design feed rate. It is hoped that improved characterization of the processes occurring in a rotary kiln will allow future designers to prevent the generation of puffs without reducing the feed rate or sacrificing the ability to feed containerized wastes.

DESCRIPTION OF RESEARCH APPROACH

When studying such a complex process as rotary kiln incineration, one needs to take a broad approach because the processes involved are complex and ultimately interrelated. Insight gained in studying one aspect of the overall process is often invaluable in understanding other aspects. Even at the current state of knowledge, however, there are probably phenomena occurring in rotary kiln incinerators that are completely unknown and unexpected, yet which strongly influence the overall process. If one always chooses to concentrate on a single piece of the overall puzzle, then the gaps in the puzzle will never be realized and studied. It is for this reason that this research is not focused upon any single phenomena or method of experimentation. Instead, the research
efforts deal with various phenomena, such as bed motion, solids mixing, solids heating, contaminant evolution, gas flow field, thermal buoyancy, and system operational aspects such as the addition of turbulence air. The methods of experimentation include studies using a pilot-scale rotary kiln incinerator, a field-scale rotary kiln incinerator, and numerical simulation techniques. This broad study approach has provided both the detail and the realism needed to understand better the rotary kiln incineration process.

It is important to note that bench-scale studies have been intentionally omitted from this research plan. Bench-scale studies tend to cover very specific, experimentally isolated phenomena under carefully controlled conditions. These studies are extremely valuable for obtaining empirical data such as sorbent properties and waste properties. Other bench-scale studies are aimed at more complicated but still experimentally isolated phenomena such as flame mode kinetics or surface desorption kinetics. These studies generally produce data that are incorporated into sub-models of specific phenomena, for later incorporation into more general models. Bench-scale studies are effort intensive, often being designed, operated, and analyzed by one or more experimenters as their sole research effort. Clearly, in terms of the overall picture, bench-scale studies are extremely important. However, the thrust of this study covers phenomena that cannot be studied adequately with bench-scale experiments. This includes phenomena in which the effects of complex geometry are important, or where interactions between phenomena occur. This also includes new phenomena and interactions that must be identified before more detailed study is possible.

The phenomena occurring in a rotary kiln that have been chosen for study include contaminant evolution from the solids bed, mixing and heat transfer in the solids bed, and gas buoyancy and flow field. These phenomena have been singled out for emphasis in this research because they appear to be very important to the overall process of rotary kiln incineration, while being poorly characterized and understood.
GOALS AND OBJECTIVES

Overall Program Goal

The overall, ultimate goal of this research program is to develop a detailed predictive capability for rotary kiln incineration. This overall goal cannot be achieved in a single step. Therefore, the following approach is used:

- Observe important phenomena experimentally (collect data)
- Propose initial sub-models to describe observed phenomena
- Evaluate these sub-models against experimental data
- Combine these sub-models into a model capable of reliably predicting the important aspects of system performance

This approach begins with experimental observations, and indeed these play a large part in this work. The reason is that the processes involved in rotary kiln incineration are complex, and their individual contributions have not been well characterized. Sub-models are then formulated to describe the observed phenomena, and these are tested against experimental data. The final step of assembling the sub-models into a predictive model for system performance is not included in the scope of this work because much remains to be done before that can be realized. Instead, it is planned to proceed with the first three steps of the approach in order to make necessary progress toward the overall program goal. With this in mind, the following specific objectives were selected for this research.
Specific Research Objectives

Field-Scale Experimental Objectives

1. To develop, improve, and expand the field-scale test procedure used in previous experiments, in order to take more detailed and more informative measurements under better controlled conditions.

2. To perform experimental tests on a field-scale facility and record detailed continuous data from the kiln, afterburner, and stack as a function of rotation rate and turbulence air addition.

3. To reduce the data to a more usable form by ensemble averaging the data in order to eliminate the effects of individual pack randomness.

4. To determine the effects of kiln rotation rate and turbulence air addition on variables measured throughout the system.

5. To perform mass balances on the system with data from the afterburner and stack.

6. To determine evolution intervals from the measured parameters directly related to the contaminant evolution (CO₂, O₂).

7. To evaluate the potential for using continuous stack oxygen data in calculating evolution rates.

8. To determine the influence of bed motion regime on contaminant evolution rate.
Numerical Model Objectives

(9) To develop a detailed numerical model of the field-scale kiln that is capable of handling the three-dimensional asymmetrical geometry and is capable of predicting the non-uniformities observed near the kiln exit during steady state operation in the absence of waste combustion.

(10) To compare the conditions at the kiln exit plane predicted by the numerical model with those measured experimentally.

(11) To demonstrate the importance of thermal buoyancy in determining the observed non-uniformities at the kiln exit plane.

(12) To determine the effect of turbulence air addition on the flow field and the non-uniformities at the kiln exit using the numerical model.

(13) To determine the effect of leak air origin and quantity on the flow field and non-uniformities in the kiln using the numerical model.

Pilot-Scale Experimental Objectives

(14) To perform pilot-scale experiments to address the rate of mixing in the solids bed.

(15) To extract information on mixing and heating time constants, as well as bed rotation frequency, from the experimental temperature data taken at the pilot scale.

(16) To propose an empirical bed mixing model based upon the pilot-scale data.
These objectives, and the chapters in which they are discussed, are listed in Table 1.1. Chapter 3 presents the details of the field-scale experimental study, together with preliminary oxygen data obtained throughout the system. Chapter 4 presents and discusses the remainder of the experimental data and the influence of operational parameters. Chapter 5 includes calculations of contaminant evolution rates and mass balances, and addresses the influence of bed motion regime. Chapter 6 includes the formulation of a numerical model of the field-scale rotary kiln, its predictions, and its validation against experimental data. Chapter 7 presents the study of solids mixing in a pilot-scale rotary kiln, including an empirical model of this phenomenon. Chapter 8 summarizes the results of this work and gives recommendations for future work.

Table 1.1 List of specific objectives and the chapters in which they are discussed.

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CHAPTER 2

LITERATURE REVIEW

This literature survey focuses on published research directed at understanding the physical processes associated with hazardous waste incineration in a rotary kiln incinerator. This review has been divided into six categories: overview and design, field-scale rotary kiln studies, pilot-scale rotary kiln studies, mixing and heat transfer studies, scaling studies, and modeling studies. For brevity, studies dealing strictly with combustion kinetics have not been included.

OVERVIEW AND DESIGN STUDIES

Oppelt (1981) presents an early review of incineration as an option for controlling hazardous wastes. He presents incineration as an effective alternative to other disposal methods because it efficiently destroys the waste. He briefly discusses the recent (as of 1981) Federal regulations imposed on incinerators as a means of ensuring that they are well designed and efficiently operated. The regulations require the owners and operators of an incinerator to obtain a permit that specifies the types of wastes to be incinerated. The facility must demonstrate its ability to meet three basic standards: 99.99% destruction and removal efficiency (DRE) for each principal organic hazardous component (POHC) of the waste feed (DRE=1-(mass of POHC flowing out the stack)/(mass of POHC fed into the incinerator)); 99% removal of hydrogen chloride from the exhaust gas; an emission limit of no more than 180 mg particulate matter per dry standard cubic meter of exhaust gas. The most severe operating conditions for which the incinerator can still meet
these conditions become the limiting conditions of the permit. Other topics covered in this review are: the incineration process; design and operation; and types of incinerators. The difficulty in predicting incinerator performance is discussed, particularly concerning the time/temperature history and mixing history of the waste. Improving this predictive capability is expected to help optimize new incinerator designs and reduce the cost of the trial burns for permitting.

In a later paper, Oppelt (1986) gives a somewhat more detailed review of hazardous waste incineration. He predicts substantial increases in the use of incineration as legal restrictions on land disposal are increased. He covers current practices, surveying current incinerators regarding their type, conditions of operation, and their performance. Analysis of the then current data revealed that no absolute level of combustion temperature, mean gas phase residence time, or carbon monoxide concentration could be correlated with achievement of 99.99% DRE. In incinerators achieving the DRE requirements, residence times ranged from 0.1 to 6.5 seconds, temperatures ranged from 648°C to 1450°C, and carbon monoxide levels ranged from 5ppm to 600ppm. He concludes that the relationship between operating conditions and performance is facility specific, and concedes that it is currently impossible to specify absolute operating parameters that will guarantee in advance a 99.99% DRE for a particular waste. He mentions efforts to increase a data base of trial burn data for predictive capability, and emphasizes efforts to identify easily monitored process variables, such as carbon monoxide concentration, for use as real time indicators of system performance.

Finally, Oppelt (1987) suggests that of all "terminal" treatment technologies, incineration is capable of the highest degree of destruction and control for the broadest range of hazardous waste streams. He contends that there is a substantial amount of design and operational experience for hazardous waste incinerators, and he covers this information in some detail. Included is an extensive review of regulations, current
practices, various types of incinerators, process monitoring, performance measurement, a
survey of incinerator emissions, methods of predicting and assuring performance, and
risk assessment. Among his conclusions are: available methods for predicting incinerator
performance for particular compounds do not correlate with field experience; none of the
available real-time performance indicators appear to correlate with DRE, although some of
these indicators, particularly carbon monoxide and unburned hydrocarbon concentration,
may be useful for estimating the lower bound of acceptable DRE performance; based on
the then current assessments, there appears to be little increased human health risk from
hazardous waste incinerator emissions; there is considerable public opposition to siting
and permitting of hazardous waste incinerators even though they have demonstrated
performance levels and apparently pose little human health risk.

Lee, Huffman, and Oberacker (1986) give another review of hazardous waste
incineration, including regulations, different types of incinerators with advantages and
disadvantages, types of pollution control equipment, and process monitoring and
performance measurement. Although they conclude that incineration is the best available
demonstrated technology for waste destruction, they also concede that it is not a perfect
technology, and that considerable research is needed to ensure that emissions are
adequately controlled.

Gregory (1981) discusses the many factors involved in incinerator design,
particularly those operated by Rollins Environmental Services. He covers specific
components of the incinerators' designs, including design conditions at each location in
the system. He points out that the designer is faced with a limited supply of published
data, particularly if a variety of wastes are being considered. He concludes that, in order
to meet the rigorous regulations with limited resources of design information, the design
engineer should develop a very conservative design, making a special effort to estimate
the worst possible case waste to be disposed of in the system.
Pitts and Cudahy (1984) discuss various combustion system design considerations that they consider important in the design and upgrading of hazardous waste incinerators. The design areas include discussions of nozzles, burner assemblies, flame patterns, atomization, large droplets, gas phase mixing, heat loss, refractory, waste characteristics, and thermal oxidation stability of the waste compounds. Two trial burns for rotary kiln incineration systems are also discussed. The authors also discuss the use of the EPA's pilot-scale liquid incinerator as a research tool for obtaining data on the various design considerations.

In summary, there have been a few excellent reviews of rotary kiln incineration. Unfortunately these reviews focus on the rotary kiln incinerator system as a unit, with little or no mention of the processes occurring within the rotary kiln. This is evident in the few published design studies and their rather primitive treatment of rotary kiln design. These design papers rely on rule-of-thumb methods and emphasize known processes such as burner characteristics or heat loss through the walls, while advocating large safety factors to account for the little known processes affecting overall performance.

FIELD-SCALE INCINERATOR STUDIES

Rotary kiln incinerators have become a common topic of research papers recently. Unfortunately, of the papers addressing industrial scale rotary kiln incinerator performance, virtually all of them deal with emissions measured at the stack, particularly during trial burns. Almost none have dealt with processes inside the kiln and their influence on system performance. The only exception is the work carried out at Louisiana State University by Cundy, Sterling, Lester, and co-workers.

Cundy et al. (1989a) describe the overall program goals for the rotary kiln incinerator research program at Louisiana State University. The sampling methods are described, including the use of large water cooled probes and associated equipment for taking gas samples and species measurements from within the rotary kiln. The samples
are taken in gas sample bombs for later analysis with GC techniques. Preliminary species and temperature measurements are presented for both the kiln and afterburner during the steady state incineration of liquid carbon tetrachloride atomized into the kiln.

Cundy et al. (1989b) compare species and temperature data from steady incineration of liquid carbon tetrachloride as a function of location in the system. Measurements taken at the kiln exit, the transition region, and the afterburner are compared. This work also compares measurements taken at two different vertical locations near the kiln exit plane. Large non-uniformities are observed at the kiln exit, and these non-uniformities persist into the afterburner. The addition of turbulence air appears to reduce these non-uniformities; however, it also reduces the measured gas temperatures in the upper kiln where the bulk of the waste destruction is thought to occur.

Cundy et al. (1989c) compare species and temperature data from steady incineration of liquid carbon tetrachloride at a variety of locations near the kiln exit. Large non-uniformities are observed at the kiln exit, and these non-uniformities persist into the afterburner. Some of these locations, particularly in the transition section, are characterized by oxygen concentrations and temperatures approaching ambient conditions. In spite of this, the DRE for the carbon tetrachloride during these tests was always well in excess of the 99.99% required by permit.

Cundy et al. (1989d) present species and temperature measurements obtained during the batch mode incineration of toluene-laden sorbent packs. During this study, the injection of turbulence air at ambient temperature is the only independent variable. Although the time resolution of the data is coarse, strong transients in temperature and total hydrocarbons are observed both with and without turbulence air addition. Also included in this paper is a summary of the steady state carbon tetrachloride studies, and some preliminary toluene incineration results from the pilot-scale rotary kiln at the University of Utah.
Lester et al. (1989) provide a much more detailed analysis of batch mode incineration of toluene-laden sorbent packs in a rotary kiln. Again, transients in temperature and total hydrocarbons are observed and correlated with visual observations of the flame and soot present in the kiln. Also presented are the species measurements from within the kiln and afterburner showing extremely low levels of benzene and no detectable toluene. They also discuss the repeatability of species and temperature measurements, levels of oxygen, carbon monoxide, and total hydrocarbons measured in the stack, and volatile organic sampling train results from the stack. One surprising observation is the presence of large amounts of soot in the lower half of the kiln, where oxygen concentrations are the highest. Each pack of toluene appears to produce two transients characterized by copious sooting, separated by a period of little soot but much flame. The authors suggest that the first soot cloud blocks radiation heat transfer from the flame to the solids, thus reducing the toluene evolution rate. When the soot cloud dissipates, heat transfer increases, resulting in a second transient.

Cundy et al. (1991a) discuss the incineration of xylene/sorbent packs in a rotary kiln incinerator. As in their previous studies, gas samples are drawn from within the kiln through a water cooled probe. However, in this study the samples are continuously monitored for oxygen, carbon dioxide, carbon monoxide, total hydrocarbon, and temperature. Again, vertical stratification at the kiln exit is observed, even for the transient feed. Increasing rotation rate appears to increase the magnitude of the transient excursions somewhat. The addition of turbulence inducing air apparently only dilutes species concentrations in the lower kiln, reducing the temperature slightly. In the upper kiln, the turbulence air causes no change in the observed temperature, but almost completely eliminates the transient excursions of the measured species. Video images taken during the study are discussed, and they appear to show the double transient phenomena observed during previous studies with toluene (Lester et al. 1989). The double transients are also evident in the continuous data. Based upon the visual
observations, they propose that the observed transients are associated with macroscale bed motion (disintegration and motion of packs within the bed) and not microscale bed motion (homogeneous solids bed slumping) as suggested by some others.

Cundy et al. (1991b) compare xylene and dichloromethane pack processing in a field-scale kiln study. The comparison includes the same xylene test data covered by Cundy et al. (1991a). In general, dichloromethane processing produced higher levels of carbon monoxide, total hydrocarbon, POHC, and intermediate stable product species measured in grab samples. In contrast, xylene processing exhibited only very low levels of benzene as an intermediate product. During processing with both xylene and dichloromethane, significant stratification was observed at the kiln exit. The upper kiln was characterized by relatively low oxygen levels and high temperatures, while the lower kiln exhibited the opposite conditions. Xylene combustion always appeared to occur primarily in the lower kiln. When no turbulence air was added, the xylene produced hot, buoyant, oxygen-deficient gas packets that expanded into the upper kiln, starving the natural gas support flame and resulting in uncombusted methane. In contrast, this did not occur with dichloromethane, probably because of its lower heating value. Dichloromethane decomposition products were present primarily in the lower kiln when no turbulence air was added. However, the addition of turbulence air appeared to transport these products to the upper kiln, where the low oxygen levels made destruction more difficult. Both xylene and dichloromethane exhibited evolution transients apparently related to macroscale bed motion. Finally, increasing rotation rate caused a slight increase in the magnitude of the transients for both compounds.

Cundy et al. (1991c) discuss the calculation of evolution rates and mass balances for a field-scale rotary kiln processing dichloromethane contaminated clay sorbent contained in plastic drums. Experimental data is collected during processing at two different kiln rotation rates and operation with and without turbulence air injection. Because measurements at two locations near the kiln exit show that the gas stream was
not homogeneous, several assumptions are made in the analysis. The procedure for calculating evolution rates and mass balances is the same as that presented by Lester et al. (1991), and is discussed in the scaling section of this literature review. Mass closures on the dichloromethane are 85% to 110% during operation without turbulence air and 65% to 75% during operation with turbulence air, showing a trend similar to that observed for xylene by Lester et al. (1991). The calculation of weighting factors for flow in the upper and lower kiln suggest that the bulk of the waste combustion products flow through the lower kiln during operation with no turbulence air, and through the upper kiln when turbulence air is activated. The average evolution rate for dichloromethane shows little dependence on either turbulence air addition or kiln rotation rate.

In summary, there is a dearth of published data regarding measured conditions and observed processes within field-scale rotary kiln incinerators. The only exception is the work carried out at Louisiana State University by Cundy, Sterling, Lester, and co-workers on a single rotary kiln operated by Dow Chemical. These studies have provided the only published accounts of conditions within a field-scale rotary kiln incinerator, and they have provided valuable insight into the complex processes that affect performance. A large number of published accounts of field-scale rotary kiln incinerator studies, particularly trial burn summaries, have been omitted here because they have treated the entire incinerator system as a black box, generally with temperature being the only measured condition within the rotary kiln. These studies provide very little insight into rotary kiln processes. Instead, they emphasize a trial and error approach to establishing an envelope of acceptable operating conditions.

PILOT-SCALE KILN STUDIES

Lnak et al. (1987a) describe the use of a pilot-scale rotary kiln incinerator (simulator) for measuring evolution characteristics and puff formation with batch fed solid wastes. The simulator is a 73 KW directly fired unit with a solids chamber of 0.762 m
inside diameter and 0.61 m in length. The authors use statistical response surface techniques to select test conditions for parametric studies. They select charge mass, charge surface area, kiln temperature, and waste material as the independent variables. The waste charges consist of a number of plastic rods of varying lengths to give the desired mass and surface area. The rods consist of high density polyethylene, low density polyethylene, polyvinyl chloride, and polystyrene plastics. The dependent variables are transient peak height of the total hydrocarbon analyzer sampling the kiln exhaust gas, and the total area under each transient peak. The results of the experiments are statistically analyzed to produce response surfaces of the dependent variables. The authors conclude that increasing the temperature may increase the peak puff intensity and decrease the integrated mass of hydrocarbons exiting the kiln. Both peak puff intensity and integrated mass are strong functions of the mass and surface area of the charge. The authors suggest that the formation of transient puffs results from a complicated mixture of physical and chemical processes in the kiln. The processes appear to be strongly dependent on the nature of the solid waste, the heat transfer, the rate of waste gasification, and the gas phase stoichiometry.

Linak et al. (1987b) discuss the incineration of liquids bound on solid sorbent material contained in cardboard containers. The researchers use the same pilot-scale rotary kiln described by Linak et al. (1987a). In these tests, the waste charges consist of toluene, dichloromethane, carbon tetrachloride, or No. 5 fuel oil adsorbed onto ground corncob material contained in 0.95 L cylindrical cardboard cartons. Parametric studies are performed using statistical response surface methods. The independent variables are kiln temperature, liquid charge mass, and kiln rotation rate, while the dependent variables are total hydrocarbon peak height and area. Increases in any of the three independent variables leads to increases in both of the dependent variables. Difficulties with nonlinear response of the total hydrocarbon analyzer are discussed, as well as problems determining the appropriate puff indicator (THC, CO, soot mass) for each waste species. The
speciation of the exhaust gas is reported for each of the waste species tested. The authors propose that the volatile release rate is probably controlled by heat transfer, surface exposure, vapor pressure, and heat of vaporization of the waste liquid.

Wendt and Linak (1988) propose a theoretical model to predict waste evolution and puff formation from batch loaded liquid wastes bound on ground corncob sorbent material. The proposed model relates desorption rate to vapor pressure (via the Clapeyron relationship) and to surface area. They assume that the surface area follows a fragmentation type behavior in which the solids periodically fragment to produce two pieces out of every one. The rate of fragmentation is assumed directly proportional to the kiln rotation rate. The model appears to simulate the salient features of the experimental runs, including multiple evolution peaks, but it fails to agree quantitatively without adjustment of the parameters.

Lemieux and Pershing (1989) present details of the design and construction of the pilot-scale rotary kiln simulator at the University of Utah. The solids cavity in the kiln is 0.61 m long and 0.61 m in diameter. A 73 KW coaxial translatable gas burner provides direct heating in the system. The kiln is refractory lined and is capable of temperatures up to 1650°C. An airlock gate in the exhaust end of the kiln provides access for loading charges of waste into the kiln. Charges are placed in the solids cavity with the aid of a hand-held 1.5 m long loading chute that is inserted through the gate. Removal of the solids is facilitated by a water cooled suction probe connected to a solids collection hopper, a gas heat exchanger, and ultimately to a large vacuum cleaner. The exhaust gas exiting the kiln is sampled by a variety of instruments before entering the afterburner section. Typical results are presented for zirconium oxidation in this system, and preliminary results from incineration of sorbent bound toluene are also included.

Cundy et al. (1989d) discuss the use of the Utah pilot-scale rotary kiln simulator as part of their overall study of rotary kiln incinerators (see field-scale section of this literature review). They perform a parametric study on the batch incineration of toluene
laden clay sorbent contained in paper envelopes. The independent variables are kiln rotation rate and temperature. The dependent variables are the transient responses of \( \text{O}_2 \), \( \text{CO}_2 \), CO, THC, and gas temperature. The transient responses tend to show two relatively low magnitude evolution events at low rotation rates. As rotation rate increases, these two peaks move closer together and increase in magnitude until a single large peak results. The occurrence of these peaks corresponds with the onset of combustion of the pack and the first slump of the solids, respectively, both of which expose fresh solid material. Increasing the kiln temperature from 621°C to 732°C has little effect on the transient responses.

Owens et al. (1992) perform studies on toluene adsorbed on montmorillonite clay particles. Charges of this waste are fed into the empty pilot-scale rotary kiln simulator where the toluene is vaporized without combustion and is measured in the kiln exhaust gas. The independent variables for the study are kiln wall temperature, solids fill fraction, and kiln rotation rate. The bulk temperature of the solids is measured continuously with a thermocouple immersed in the bed of solids. The time-varying desorption rate of toluene is calculated from the exhaust gas flow rate and the measured toluene concentration in the exhaust gas. These data are interpreted in terms of a surface renewal model. The model assumes that the bed is periodically well mixed, with depletion of toluene occurring on the exposed surface during the stationary intervals. This draws conceptually upon the observed slumping motion of the bed, where the surface of the solids is stationary until a slump occurs and the surface is renewed. The slumping frequency is determined experimentally as a function of fill fraction and rotation rate, and is then incorporated into the model. The rate of toluene desorption is determined by the rate of diffusion through the surface layer, which is approximated as a semi-infinite medium; an effective diffusion coefficient with an Arrhenius-type dependence on temperature is used. The resulting model has two empirical constants that are adjusted to give the best fit of the data. The temperature in the Arrhenius term is supplied by the measured bed temperature (assuming
the bed to be spatially isothermal) as a function of time. Because the model is exponentially dependent upon temperature, the predicted evolution rates are highly sensitive to the temperature of the solids. The predicted toluene evolution rates agree surprisingly well with those determined experimentally, although the two fit parameters were temperature dependent.

In contrast to most studies of field-scale incinerators, pilot-scale rotary kilns have been used to study specific phenomena occurring within the rotary kiln. Although there have been studies using pilot-scale process rotary kilns, only those used to study hazardous waste incineration have been included here. These simulators have provided valuable data, with particular emphasis on waste evolution from solids and puff formation.

**BED HEAT TRANSFER STUDIES**

Imber and Pashkis (1962) construct two heat transfer models for evaluating the assumption of well-mixed solids in kilns. One model assumes transverse well-mixed solids, resulting in a one dimensional problem. Experimentally determined heat transfer coefficients for a lime kiln are used (from the experiment with which the model predictions are to be compared). An alternative model is formulated assuming the bed is an unmixed slab of finite thermal conductivity, with the upper and lower surfaces at the experimentally measured gas and wall temperatures, respectively. Compared to the experimental data, the predictions of the well-mixed model agree well, while the unmixed model grossly underestimate the exit temperatures. The authors conclude that for conditions typical of cement and lime kilns, the well-mixed solids assumption is appropriate.

Sass (1967) presents a typical simplified model of heat transfer to wet solids in a rotary kiln. The model consists of differential equations to predict axial profiles of temperature and concentration. Heat transfer coefficients are evaluated using correlations
available in the literature. The model shows good agreement with experimental measurements of gas and solid temperatures in an industrial cement kiln and gas temperatures in an iron ore process kiln. The good agreement may be attributed to the adjustment of several poorly characterized coefficients to obtain the best fit of the data.

Kern (1974) presents a heat transfer model of a rotary heat exchanger that includes the usual assumptions of well-mixed gas and solids at each axial cross section. However, in order to account more accurately for the regenerative heat transfer from the wall, a relatively simple wall model is solved to yield an analytical expression for the circumferential wall temperature distribution. The model is used to predict temperature profiles as a function of length, rotation rate, and temperature change, but is not compared to experimental data.

Wes, Drinkenburg, and Stemmerding (1976) present a model for heat transfer in a horizontal drum reactor. The heat transfer model is based upon a thermal penetration into stationary solids at the wall, followed by mixing while traversing the free surface of the bed. The effective wall to solids heat transfer coefficient is then predicted based upon the analytical solution for transient conduction into a semi-infinite solid. Solids temperature and heat transfer coefficients are compared to those determined experimentally in starch heaters, and the results appear to agree very well.

Ghoshdastidar, Rhodes, and Orloff (1985) present a heat transfer model for a rotary kiln incinerator burning solid Plexiglas waste. The model uses a zonal technique to account for radiation heat transfer, a finite element technique to account for circumferential wall temperature variation, and the solids are assumed transversely well mixed. A first order kinetic relationship is used to predict the waste volatilization and its subsequent combustion. Temperature profiles and solids burnout are predicted for several different fill fractions, but no comparison is made to experimental data.

A group at the University of British Columbia, Vancouver, has done extensive work on heat transfer and bed motion in rotary kilns. The group, including Barr,
Brimacombe, Gorog, Henein, Tscheng, and Watkinson, has focused on conditions associated with metal ore processing and not waste incineration. However, their extensive work has included both theoretical and experimental aspects, and they have produced valuable data using a pilot-scale rotary kiln facility. A review of their publications follows.

Brimacombe and Watkinson (1978) introduce the research program on rotary kiln reactors at the University of British Columbia. They acknowledge that heat transfer is often the most important part of rotary kiln processing, yet it is poorly understood and there is little controlled experimental data available. They attribute this to the difficulty in making measurements in a rotating vessel. They observe that design of rotary kiln processes (as of 1978) is done using rule-of-thumb methods in lieu of predictive models. They discuss the U.B.C. pilot rotary kiln, which is 5.5 m long, 41 cm in diameter, with an 8 to 104 kw support burner in a directly-fired, counter-current flow configuration. Solids feed is accomplished via a screw mechanism to simulate the steady feed typical of process rotary kilns. The facility is heavily instrumented, with many thermocouples measuring the temperatures of the kiln shell, kiln refractory, solids, and gas. Data are transferred from the rotating thermocouples to data recording equipment via a series of slip rings and contact brushes. A series of experiments is described, and the data reduction methods are discussed. The objective of the tests is to calculate heat fluxes across interfaces in the system over a range of operating conditions. These heat fluxes are calculated assuming: gases and solids move in plug flow; radiative heat flux in the axial direction is negligible; at any axial location, the gas and solids are each characterized by a single temperature (only temperature gradients in the axial direction are considered). These results and their analysis follow in the second paper of the series.

In the second paper of the series, Watkinson and Brimacombe (1978) present the experimental heat fluxes in the pilot-scale kiln and compare them to predictions based upon simple models. For the gas to refractory wall heat flux, experiments and predictions
agree very well. For gas to bed heat flux, predicted values are an order of magnitude smaller than experimental values. The authors describe bed motion as either slumping or rolling, and estimate coefficients for gas to solids heat transfer for each motion regime. They also present a bed behavior diagram that predicts the motion regime for a particular solid in the pilot kiln as a function of fill fraction and kiln rotation speed. They observe that rolling bed motion is characterized by larger heat fluxes than slumping motion. They use a two resistance approach to derive heat transfer coefficients for both the gas side and burden side of the gas-solids interface. In an appendix, the authors consider heat flux across the bed-wall interface. Because the measured wall temperatures and bed temperatures were only slightly different, this mode of heat transfer was neglected in the preceding calculations. They use penetration theory to estimate heat fluxes between the wall and the solids, and conclude that they are less than 13% of the total heat flux to the bed and are therefore negligible. They reach a similar conclusion regarding radiative heat flux between the wall and the free surface of the solids under the conditions of this study.

Tscheng and Watkinson (1979) perform a study on convective heat transfer in a rotary kiln. They calculate heat transfer coefficients from experimental data using a pilot-scale rotary kiln with the following assumptions: both the gas and solid phases exhibit plug flow with uniform (but different) temperatures at each axial location; the local wall temperature does not fluctuate as it is covered by the bed and subsequently uncovered; the bed surface is planar, with an area equal to its chord length times the kiln length. In this study the kiln is not fired, heat being supplied by hot air flowing through the kiln, resulting in negligible radiation heat transfer. In order to calculate convective heat transfer coefficients between the gas and solids, heat transfer between the solids and wall is calculated using a correlation that the authors construct based upon literature data. The correlation relates the solids-wall Nusselt number to \( (nR^2 \beta / a)^{0.33} \) where:

\[
n = \text{rotational speed (rev/sec)}
\]

\[
R = \text{kiln radius (m)}
\]
\[ \beta = \text{central angle of sector occupied by the solids bed (rad)} \]

\[ a = \text{thermal diffusivity of the solids (m}^2/\text{sec)} \]

The data approach limiting values for small particle size, and the correlation applies only in the limit of small particles. The researchers conclude that the gas to solids heat transfer coefficient is an order of magnitude higher than that from the gas to bare wall. They attribute this to the large surface area of the particles on the surface, and to the effect of lateral velocity of the solids as they move down the inclined surface. Correlations for gas-wall and gas-solids heat transfer coefficients are fit to the data and presented. It is observed that solids throughput and kiln inclination angle have no influence on heat transfer coefficients, and the fill fraction does not influence the gas-wall heat transfer coefficient. The effect of particle size is negligible within the narrow range of particle sizes tested.

Gorog, Brimacombe, and Adams (1981) perform a theoretical study on radiative heat transfer in rotary kilns. Radiation is thought to be the dominant mode of heat transfer in field-scale rotary kilns due to the high temperatures typical of operation. The authors construct a radiative heat exchange model that accounts for the kiln and bed geometry, includes emission, absorption, and diffuse reflection from the solid surfaces that are assumed to be gray, and treats the gas as a non-gray gas with distinct emission/absorption bands. The resulting equations are numerically integrated, and results are presented in chart form. They compare the results to those obtained with a simpler gray gas approximation solution using a resistance network approach. They conclude that since the gases in a typical kiln contain much CO\textsubscript{2} and H\textsubscript{2}O, the gas phase should be treated as a real gas and not as a gray gas. Predictions show that for kiln wall and solids reflectivities greater than 0.2, the gray gas assumption will lead to heat exchange more than 20\% in excess of the real gas model. They show that gas-solids or gas-wall heat exchange occurs primarily within a ±0.3 kiln diameter axial distance because the gas participates strongly in the radiative heat transfer, allowing the axial temperature gradients
to be treated as a series of isothermal zones with little error. Gas radiation that is reflected from the walls and solids tends to be reabsorbed by the gas, so reflection at these wavelengths only influences the heat transfer locally. Radiant exchange between the solids and the kiln wall occurs primarily within an axial distance of ±0.75 diameters, so even in the clear gas wavelength band the assumption of axial isothermal zones may be very good. Charts are presented which may be used to estimate radiant heat transfer in a rotary kiln as a function of kiln diameter, gas composition, temperature, and fill fraction.

Gorog, Adams, and Brimacombe (1982) also develop a mathematical model to evaluate regenerative heat transfer in rotary kilns. Regenerative heat transfer is the process in which heat is transferred from the hot gas to the exposed kiln walls. The kiln rotates until this part of the wall is covered by the solids bed, and heat is transferred from the wall to the bed. The cooled wall then rotates until it is exposed to the gas again and picks up more heat. The mathematical model uses a finite-difference method to simulate the temperature distribution in the kiln wall. Radiation is treated using a zonal method assuming gray surfaces and gray gas. The solids bed and gas are assumed isothermal at each axial location. Heat transfer coefficients between the gas and walls, gas and solids, and solids and walls are predicted using the correlations developed by their co-workers (Tscheng and Watkinson 1979). The model is used to evaluate the effect of several process variables on the regenerative and total heat flow to the solids. The authors conclude that the kiln wall temperature distribution and total heat flow to the solids is relatively insensitive to process variables such as kiln rotation rate, fill fraction, wall thermal properties, emissivities, or heat transfer coefficients. They reason that changes in the process variables have opposing effects on the different modes of heat transfer, resulting in overall insensitivity to the process variables. Of course, these results apply only over the range of conditions simulated in this study. Other conclusions of note are drawn from the study. The penetration of cyclic temperature variation into the kiln walls rarely exceeds 1.5cm, and the magnitude of the variation in wall surface temperature is
between 30 K and 90 K. At the burner end of the counter-flow kiln, 60% to 80% of the heat transfer to the bed is via radiation, while at the relatively cool solids feed end, only 30% is via radiation. The authors construct a greatly simplified resistance analog model that assumes the kiln wall is also isothermal at each axial location, as justified by the results of the more elaborate model. This simplified model is able to predict axial wall temperature profiles and heat flows within 5% of the more elaborate model predictions for the conditions of this study.

Henein, Brimacombe, and Watkinson (1983a) present an experimental study on bed motion in a pilot-scale kiln and in rotating cylinders. Experiments are performed using a variety of granular solids in different diameter cylinders as rotation rate and fill fraction are varied. The type of bed motion resulting, generally slipping, slumping, or rolling in this study, is plotted against bed depth and rotational speed to create a bed behavior diagram for a given solid material and cylinder diameter. This characterization is needed for better estimation of heat transfer coefficients in the system and this study is discussed in more detail in the Bed Motion and Mixing section of this literature review.

Henein, Brimacombe, and Watkinson (1983b) discuss modeling of bed motion in rotary kilns. Their objective is to develop a fundamental basis for the behavior observed by Henein, Brimacombe, and Watkinson (1983a). The authors present a semi-empirical model for predicting the transition from slumping to rolling bed motion. This paper is also discussed in more detail in the Bed Motion and Mixing section of this literature review.

Gorog, Adams, and Brimacombe (1983) present a mathematical model for estimating temperatures and heat flows in the flame zone of a directly fired rotary kiln. This model is to complement the work done on non-flame zones in a kiln (Gorog et al. 1981, 1982). The authors use a zonal analysis consisting of resistance analog networks in each zone to model the heat transfer. In each axial zone, the walls, gas, solids, and flame are each assumed to be isothermal, and axial radiation is neglected. The flame,
wells, and solids are treated as radiatively gray with the emissivity of the flame taken as 2/3 of the peak emissivity of the flame based upon the carbon to hydrogen ratio of the fuel. The flame is taken to be a constant diameter cylinder on the axis of the rotary kiln, with a length estimated from burner and fuel type. The gas surrounding the flame is assumed to be air and thus does not participate in the radiation heat transfer. The model is used to study the influence of process variables on heat transfer, but the results are not compared to experimental data. The use of a fuel yielding a more emissive flame increases the heat flow to the solids while decreasing the flame temperature. For a natural gas flame, preheating the secondary air increases the flame length resulting in greater heat transfer to the solids, while increasing the primary air flow rate has the opposite effect. Oxygen enrichment of the primary air reduces the flame length but increases heat transfer to the solids because the flame temperature is increased. The results apply only to the flame zone of a kiln, and any subsequent heat transfer must be modeled using the non-flame models while matching temperatures and flow rates at the interface.

Barr, Brimacombe, and Watkinson (1989a) present the results of a series of experimental heat transfer studies in a pilot-scale rotary kiln. These studies are more extensive than those described by Brimacombe et al. (1978), and the facility was more heavily instrumented. The objective is to obtain pilot-scale data detailed enough to compare with heat transfer model predictions. The authors observe that the solids are heated very rapidly in the first 1.5m of the kiln, followed by declining net heat input to the bed. In beds undergoing endothermic reactions, at the location of reaction onset the net heat input to the bed increases sharply as does the thermal transients of the inner refractory surface. Under conditions of the study, regenerative heat transfer from the wall to the bed amounts to a maximum of 60% of the heat transfer through the free surface of the bed. Negative regeneration, with the bed transferring heat to the wall, is often encountered beyond the kiln midpoint except for the case of endothermic reaction in the
bed. The bed temperature and kiln wall temperature are observed to be closely coupled, even when endothermic reactions occurred.

Barr, Brimacombe, and Watkinson (1989b) present a detailed heat transfer model for a rotary kiln, and compare predicted results with experimental data. The model uses a ray tracing technique to model radiant heat exchange between the wall, the solids, and the gas. The model treats the spectral absorptive behavior of the gas using three gray gas bands and a clear band. Reflection from the solid surfaces is accounted for, while the presence of a flame is not addressed. Conduction in the walls and solids is modeled using a finite difference scheme, and heat transfer from the wall to the solids is simulated directly as transient conduction rather than using a convection coefficient. The model is intended to simulate a single axial zone of a kiln, a series of such zones being necessary to model the entire kiln. The comparison with experimental data proved difficult as the model required input values for gas temperature and bed temperature, and it showed extreme sensitivity to the input bed temperature. Since the experimentally measured bed temperatures are only accurate within ±25 K, the model is run for several different bed temperatures within that range, and these runs are all compared to the experimental data. The resulting predictions appear to agree well with the experimental data for a wide range of solids materials and conditions, although the methodology is not rigorous. The authors conclude that the model works and use it to predict heat transfer in a simulated 4 m diameter prototype kiln. They conclude that the essential features of the interaction between heat transfer processes are the same at each scale.

Owens et al. (1991) discuss a transient temperature model and a series of experimental pilot-scale incineration studies of moist clay sorbent that they compare to the model. The experimental study focused on four independent variables: bed fill fraction, kiln rotation rate, kiln wall temperature, and moisture content of the sorbent. The bed temperature is the single dependent variable. The model consists of a thermal resistance network to simulate an indirectly fired rotary kiln, which approximates the conditions of
low temperature operation in the directly fired kiln simulator. The radiation heat transfer is accomplished using gray gas and gray wall approximations, while the heat transfer coefficients are estimated using correlations available in the literature. The usual assumptions of axial plug flow for the gas, transversely well mixed solids and gas, and axial zones dividing the kiln into segments are used. The resulting model predicts transient heating of the solids in the simulator because the simulator allows only batch processing; solids do not flow axially through the system. The heating of the moist solids is treated in three stages; initial heating to 100°C, isothermal evaporation of water at 100°C, and final transient heating of the dry bed. The authors compare the model predictions to measured temperature data from dry sorbent and get generally good agreement, particularly at higher fill fractions, higher rotation rates, and lower temperatures. The experimental trends caused by variation of the independent variables are all predicted by the model. Predictions for moist sorbent are qualitatively similar to the experimental results although the model tends to overpredict the overall heating rate. The experimental data does show an approximately isothermal period at 100°C while the moisture evaporates. The model is then used to predict thermal time constants, and simple scaling laws for heat transfer are developed on this basis. The scaling laws differ for convection dominated heat transfer and radiation dominated heat transfer, and differ further if moisture vaporization is occurring. The result is a set of scaling laws that are unlikely to be all matched for two different sized kilns. The relative importance of the radiation and convection heat transfer is presented, with convection heat transfer more important at low temperatures. For a typical set of conditions, the convective heat transfer is more than twice as large as the radiation heat transfer for kiln wall temperatures below 700 K.

In summary, substantial work has been done on heat transfer to the solids in a rotary kiln, particularly through the use of pilot-scale process rotary kilns. Most of this work has emphasized process kilns such as lime kilns or ore oxidation kilns, but some of
the results may apply equally well to hazardous waste incinerators. Because of this emphasis, these studies tend to focus on axial temperature profiles during steady-state solids feed. The paths of heat transfer to the bed have been well documented as: radiative exchange with the support flame, gas, and kiln walls; convection with the gas; and regenerative heat transfer via convection and radiation to the bare kiln wall followed by conduction between the covered kiln wall and the bed. Correlations are available for estimating various heat transfer coefficients but they are not very accurate. Mixing augmented heating of freshly fed solids has not been addressed, probably because of the emphasis on continuously fed process kilns.

BED MOTION AND MIXING STUDIES

Danckwerts (1953) discusses mixing of all types of materials from a very fundamental perspective. Although the majority of the work is not applicable to mixing in a rotary kiln, a dimensional analysis is presented which may apply to any mixing system. The author describes mixedness of a system in terms of a volume scale of segregation compared to the total volume of the system, and its scaling groups are:

\[
\frac{v}{L^3} = \text{function} \left[ \frac{u L \rho}{\mu}, \frac{u t}{L}, \frac{u^2}{gL} \right]
\]

\(v\) = volume scale of segregation

\(L^3\) = total volume of the mixing system

\(u L \rho / \mu\) = Reynolds number

\(u t / L\) = scale factor for mixing time

\(u^2 / g L\) = Froude number

The Reynolds number for flow of solid particles is not clearly defined. The mixing time scale factor could be useful in scaling experimental mixing data from simulators to field-scale kilns. The appearance of the Froude number is also of interest because it has been
used for similarity of bed motion regimes in rotary kilns (Henein et al. 1983a). This analysis neglects molecular diffusion, which is not present in mixing of solid particles, and it presumes that some aspect of the mixing motion is influenced by gravity.

Lacey (1954) presents a theoretical discussion of solid particle mixing in a variety of systems. He uses a statistical approach to define mixedness as a function of sample variance of the mixture concentration. He states that regardless of the mixing mechanism, all mixing follows an exponential rate relationship of the form:

\[ M = 1 - \exp(-kt) \] (2.2)

- \( M \) = degree of mixedness, where unity is perfectly mixed
- \( k \) = rate constant
- \( t \) = time

This relationship holds because all mixing processes tend toward an equilibrium state that can only be approached asymptotically. Several more detailed theories are discussed, along with their implications regarding the rate constant. The diffusion mixing theory is of special note as it is applied to axial mixing in a horizontal rotating drum mixer. The transverse mixing in such a system is said to be very rapid compared to the axial mixing. An analytical solution based upon Fick's second law of diffusion is presented which relates concentration to axial position, time, and a diffusion coefficient. The author concludes that the experimental data available is too limited to discriminate between any of the theoretical mixing models because they all predict similar relationships.

Gayle and Gary (1960) present a study on axial mixing of solids in a horizontal rotating drum. For the experiments, solid particles of different colors were placed in a small drum in axial compartments separated by dividers. The dividers were removed, rotation was started, and after a specified number of revolutions the solids were sampled from axial locations in the drum. The particles in the samples were separated by their
color and counted. A segregation index was calculated for the entire mixer based upon the chi-square values of the color distributions in the samples. The data are plotted, and show a linear relationship for:

\[
\frac{1}{S} = 1 + k \frac{D^{1.45} R}{L^2}
\]  

(2.3)

\begin{itemize}
    \item \(S\) = degree of segregation
    \item \(k\) = rate constant
    \item \(D\) = diameter of mixing drum
    \item \(R\) = number of revolutions of the mixing drum
    \item \(L\) = length of the mixing drum
\end{itemize}

It should be noted that since the degree of segregation is calculated for the entire system, it is not a local property. Thus, this model cannot be compared directly to an axial diffusion model that predicts concentration of particles as a function of distance from the interface and number of drum rotations.

Carley-Macauley and Donald (1962) perform a study of solids mixing in a variety of tumbling mixers including a horizontal cylinder. They define mixing in terms of the variance of local samples. The solids are distinguished by two different colors, and the proportions of the colors are measured in small samples taken at various locations within the mixer and times after the onset of mixing. The results are plotted with the variance logarithmically against the number of revolutions of the mixer. This is equivalent to an exponential relationship obtained from a first order rate process, with the slope of the resulting straight line being the decay constant. For the horizontal cylinder, the relationship was indeed a straight line, but for other mixer configurations such as an off-axis cylinder, the plots yielded variable decay constants. The authors make an effort to determine the effect of the initial positions of the two colored phases on the mixing rate, finding only a minor influence on the decay constant in any particular direction. They
find that for transverse mixing in a horizontal cylinder, the decay constant is approximately 3 revolutions, while for axial mixing the constant is approximately 2500 revolutions. They note that mixing along an inclined axis is characterized by a decay constant that begins at the smaller value but approaches the larger value after sufficiently many revolutions. This means that both axial and transverse mixing occur together along the skewed axis, and systems that show variable decay time constants may actually consist of combinations of distinct mixing processes. The authors do not thoroughly address the effect of fill fraction on their results, although for the horizontal cylinder, increasing the fill fraction from 30% to 50% very surprisingly caused the decay constant to decrease from 2.8 to 2.6 revolutions.

Carley-Macauley and Donald (1964) present a further investigation into mixing of solids in tumbling mixers. The degree of mixing is characterized as in the first paper in their series, and the mixing time constants are determined in the same fashion as before. They obtain indeterminate results for the influence of mixer rotational speed on the mixing time constant. Contrary to the first paper, they find that the transverse mixing time constant (in units of mixer revolutions) increases rapidly and nonlinearly as the fill fraction is increased. In going from a 25% to a 50% fill fraction, the time constant increases from 2 to 15 revolutions. Variations in mixing time constant due to particle size are indeterminate. The authors accurately describe rolling bed motion in the horizontal cylinder, as well as cascading, cataracting, and centrifuging. The motion of individual particles is observed as they circulate through the bed, and the authors note that mixing only occurs when the particles enter the moving layer sliding down the free surface. They surmise that the degree of mixing is related to the amount of circulation through this moving layer, but they fail to test this by plotting mixedness against number of rotations of the bed rather than relying on rotations of the entire cylinder as the dependent variable.

Lehmberg, Hehl, and Schügerl (1977) perform a study on transverse mixing and heat transfer in horizontal drum reactors. They begin by characterizing the motion of
particles in the bed during slumping or rolling behavior. Using colored tracer particles they observe qualitatively the process of transverse mixing, and their photographs are very informative. To quantify the mixing rates they place hot solids on a cold bed and allow them to mix. A stationary thermocouple located in the bed registers alternately cold or hot conditions as the temperature difference decays to zero. A log plot of the magnitude of the fluctuations yields a straight line with a slope equal to the decay time constant. They report decay time constants between 6.4 and 4.3 seconds at rotation rates between 5 and 15 rpm, compared to a measured value of 60 seconds for no rotation and a calculated time of 0.16 seconds if the particles were instantaneously mixed and only interparticle conduction occurred. They do not address the effect of rotation rate or fill fraction directly on mixing, rather they use the thermal heating time constants to calculate solids-wall heat transfer coefficients assuming that the bed is well mixed. They determine that the heat transfer coefficients are dependent upon the intermittent contact time for the solids against the wall, and upon the particle size. An attempt to model the heat transfer using a penetration depth approach with independently measured material properties overpredicts the solids-wall heat transfer coefficient by about a factor of two. An improved model allowing an air film resistance between the wall and solids is constructed, but no experimental verification is possible because the experimental data are used to determine the film resistance.

Henein, Brimacombe, and Watkinson (1983a) present an experimental study on bed motion in a pilot-scale kiln and in rotating cylinders. Experiments are performed using a variety of granular solids in different diameter cylinders as rotation rate and fill fraction are varied. The type of bed motion resulting, generally slipping, slumping, or rolling in this study, is plotted against bed depth and rotational speed to create a bed behavior diagram for a given solid material and cylinder diameter. The experiments show that the transition from slumping to rolling bed motion is favored by higher fill fractions, spherical rather than irregular particles, smaller particles, materials with a smaller static
angle of repose, and larger cylinder diameters. Similar bed behavior with particles of the
same shape but different sizes and contained in cylinders of different diameters requires
similarity in fill fraction and modified Froude number. The modified Froude number is:

\[ \text{Fr}' = (\omega^2 R/g)(D/d_p)^{0.5} \]  

(2.4)

\[ \omega = \text{kiln rotation rate} \]
\[ R = \text{kiln radius} \]
\[ g = \text{gravitational acceleration} \]
\[ D = \text{kiln diameter} \]
\[ d_p = \text{particle diameter} \]

The experimental data show that plotting bed motion transition against fill fraction and
modified Froude number will do a good job of collapsing the data from different solids
materials into a single bed motion diagram. The authors then characterize each mode of
bed motion and how it is affected by other variables. In slumping bed motion, the
maximum angle of bed inclination is only weakly dependent on rotational speed, while the
shear angle is independent of rotational speed and bed depth, but decreases with smaller
diameter particles. The slumping frequency increases for greater rotational speed and
smaller particle sizes, but is unaffected by bed depth. In a rolling bed, the dynamic angle
of repose is unaffected by rotational speed or bed depth, but it decreases with smaller
diameter particles.

Henein, Brimacombe, and Watkinson (1983b) discuss modeling of bed motion in
rotary kilns. Their objective is to develop a fundamental basis for the behavior observed
by Henein et al. (1983a). The authors present a semi-empirical model for predicting the
transition from slumping to rolling bed motion. The model shows that the transition is a
function of Froude number, fill fraction, size of the shear wedge, the minimum shear
wedge, the shear angle, and the cylinder diameter. It should be noted (the authors do not)
that their model development cannot account explicitly for particle size although the particle size may influence the shear wedge and shear angle. Relatively good predictions are obtained with the model as compared to experimental data. Transitions to other modes of bed motion are also modeled, including slipping, cascading and cataracting, and centrifuging. A detailed characterization of slumping motion is also presented.

In recent years, much progress has been made toward characterizing the motion and mixing of solids in rotary kilns or rotary drums. The regimes of motion have been well documented and even modeled. Mixing has been studied in both the axial direction and the transverse direction, and some experimental data has been presented. With relatively sparse data, no correlations or models have been developed which can predict the rate of mixing in either direction as a function of operating conditions and material properties.

**SCALING AND EMPIRICAL KILN MODELS**

Saeman (1951) presents the theoretical development of equations predicting transport time and volumetric transport rate of solids through a rotary kiln. For kilns with relatively small fill fractions, the time of passage of solids is:

\[ t = \frac{L \cdot \sin(\theta)}{2\pi R n \phi} \]  \hspace{1cm} (2.5)

- \( t \) = time of passage of solids through the kiln
- \( L \) = kiln length
- \( \theta \) = angle of repose of bed material (radians)
- \( R \) = kiln radius
- \( n \) = rotational speed of kiln (revolutions/minute)
- \( \phi \) = axial slope of the kiln (radians)
This equation applies only for beds thin enough to assume that the radius from the kiln axis to the bed surface is approximately $R$. For a kiln with a larger fill fraction, the volumetric transport rate is:

$$q = \left(4 \pi n / 3\right) \left( \phi + \psi \cos(\theta) \right) \left( R^2 - r^2 \right)^{1.5} / \sin(\theta)$$  \hspace{1cm} (2.6)

$q = \text{volumetric transport rate}$

$\psi = \text{axial slope of the bed surface (radians)}$

$r = \text{radius from the kiln axis to the bed surface (} R \text{ - maximum bed thickness)}$

The transport time is:

$$t = L \cdot A / q$$  \hspace{1cm} (2.7)

$A = \text{cross sectional area of the bed}$

The authors present further equations and considerations for kilns with constrictions and for tapered kilns. The theoretical equations are compared to experimental data reported by other researchers, and the agreement appears very good. A practical observation of this work is that the maximum volumetric transport rate for a given kiln is obtained when operating at a 50% fill fraction.

Luethge (1951) presents some short-cut scaling formulas for rotary kilns. The analysis is based upon many assumptions, including geometrically similar kilns with the same fill fraction, the time-temperature history of the solids is assumed to be the same, the auxiliary heat exchange equipment on the kilns must be comparable, and heat loss through the kiln wall is negligible. These scaling formulas are based primarily upon the solids bed surface area and its volume as they relate to the variables of concern. For optimum production:
\[ Q = k \cdot D \cdot L \]  \hspace{1cm} (2.8)

- **Q** = optimum production rate (mass / time)
- **D** = inner diameter of the kiln
- **L** = length of the kiln
- **k** = scaling constant

The proper diameter for equivalent dust pickup per mass of product is:

\[ D = k' \cdot L \]  \hspace{1cm} (2.9)

- **k'** = scaling constant

The proper rotational speed of the kiln to achieve the optimum production is:

\[ S = \frac{k'' \cdot Q}{D^3} \]  \hspace{1cm} (2.10)

- **S** = kiln rotational speed (revolutions / time)
- **k''** = scaling constant

If the mass production rate is held constant, the change in fuel usage for a different sized kiln is:

\[ F = \frac{k'''}{D \cdot L} \]  \hspace{1cm} (2.11)

- **F** = fuel usage per unit mass of product
- **k'''** = scaling constant

The scaling equations are reportedly tested against experimental data with good results, although the data are not given.
Williams, Becker, and Girovich (1988) present a physical flow simulation of a rotary kiln incinerator, emphasizing on the afterburner section. They describe a transparent scale model that uses smoke to facilitate flow visualization. Gas velocities are maintained such that Reynolds numbers are equal to those of a proposed field-scale incinerator. The model is used to estimate gas residence time in the afterburner chamber. Various secondary burner and baffle arrangements are evaluated. The average residence time of smoke in the afterburner chamber was maximized using a burner and baffle arrangement that produced a strongly recirculating flow, providing substantial back-mixing. The authors conclude that the flow model provides residence times that are more accurate than those obtainable using conventional sizing techniques, although they do not claim that the predictions will agree with the behavior of the field-scale unit, and no experimental field-scale results are presented for comparison.

Lester et al. (1991) discuss scaling of contaminant evolution rates from solids beds in rotary kilns. Experiments conducted at the pilot scale are discussed. These experiments involved the incineration of toluene adsorbed on clay particles charged directly into the rotary kiln simulator. The combustion of each charge produced CO\textsubscript{2} that was measured as a function of time. By calculating the amount of toluene necessary to produce the CO\textsubscript{2} flow rate at any instant, the time resolved toluene evolution was inferred. From this, the integrated toluene evolution was calculated, and the final quantity evolved was compared to the quantity known to have been in the charge to get a mass balance on toluene. The integrated toluene evolution curves are then presented. Experiments conducted at the field scale are also discussed. These experiments involved the incineration of xylene adsorbed on clay particles contained in plastic drums. The analysis used to obtain integrated xylene evolution curves and xylene mass balances is similar to that of the pilot scale, with the following complication. The CO\textsubscript{2} responses were measured at two locations near the kiln exit, and due to the non-uniform conditions there, different CO\textsubscript{2} responses were obtained at each location during similar operating
conditions. This difficulty was circumvented by assuming the upper and lower CO\textsubscript{2} measurements each represent a plug flow of combustion gas, and weighting factors were used to represent their relative flow rates. Weighting factors were calculated based upon baseline values (operation with no xylene fed into the system, only the steady support burners supplying heat and CO\textsubscript{2}) of temperature and CO\textsubscript{2} at each location. The weighting factors were then used to calculate the overall xylene evolution from the bed using the two measured CO\textsubscript{2} responses. The integrated xylene evolution showed mass closure of approximately 85\% during operation with no turbulence air addition, but only about 55\% closure during operation with turbulence air addition. The integrated xylene evolution curves demonstrated substantial variability at the beginning and end of the evolution process, making comparisons of time for evolution quite difficult. In order to reduce the effects of this variability, a quantity called the "evolution interval" is defined as the time required for the middle 80\% of the ultimate contaminant evolution to occur. Evolution intervals are calculated for operation at each of two experimental kiln rotation rates, and similar evolution intervals are calculated for the pilot-scale data. The authors demonstrate that the evolution interval is directly proportional to the bed thickness, using kiln simulator data. They base this result on the assumption that the bed may be treated as a well-mixed, thermally lumped system in which the rate of heating of the bed will be proportional to the volume to surface area ratio. This ratio, for an infinite slab geometry, is the thickness of the slab. Since the bed in a kiln at relatively small fill fractions can be approximated as a slab, the rate of heating should be directly proportional to the bed thickness. Further assuming the heat transfer to the bed will directly influence the evolution of waste, they conclude that the evolution interval should be directly proportional to the bed thickness, and the experimental data do support this conclusion. Based upon this, they scale all field- and pilot-scale data to the same equivalent bed thickness (4.2 cm). Next, they contend that the evolution interval is a strong function of temperature. Assuming that the evolution rate is proportional to the vapor pressure of the
contaminant, and assuming the vapor pressure follows the Clapeyron equation, they conclude that the natural log of the evolution interval should be proportional to the inverse of the absolute temperature as:

\[ \ln(\text{EI}) = \frac{1}{T_{\text{abs}}} \]  \hspace{1cm} (2.12)

**EI** = evolution interval (seconds)

**\(T_{\text{abs}}\)** = absolute temperature

This temperature is the final temperature attained by the desorbing bed. In practice they substituted the wall temperature of the pilot-scale kiln and the gas temperature in the field-scale kiln. Finally the authors proposed that the evolution interval will be influenced by the motion of the solids bed. Following the work of Henein et al. (1983a, 1983b), they propose that the evolution interval should scale with the modified Froude number:

\[ \text{Fr}' = (\omega^2 R/g)(D/d_p)^{0.5} \]  \hspace{1cm} (2.13)

**\(\omega\)** = kiln rotation rate

**R** = kiln radius

\(g\) = gravitational acceleration

**D** = kiln diameter

**d_p** = particle diameter

They summarize the scaling of the evolution interval, once corrected to a reference bed thickness, as:

\[ \ln(\text{EI}_{\text{corrected}}) = \text{function of } \left( \frac{1}{T_{\text{abs}}}, \text{Fr}' \right) \]  \hspace{1cm} (2.14)
They then plot $\ln(E_{\text{corrected}})$ against $1/T_{ab}$ and draw lines of constant $Fr'$ through the data. The proposed relationships are clear with the pilot-scale data, while the trends observed in the field-scale data are only qualitatively similar. The relatively sparse data (only 4 data points for the field scale) contributes to the somewhat ambiguous results. Considering the severe assumptions made in the analysis, the results are surprisingly good.

Crude relationships have existed for many years for scaling process rotary kilns over relatively small size and performance ranges. More detailed scaling models have been developed recently which appear to show good results over large size ranges, however, much more work in this area is needed. Semi-empirical models for predicting solids throughput in process rotary kilns have also existed for many years. Flow visualization and similarity have seen limited use in simulating the gas phase flow and mixing. Currently, no empirical models exist which accurately predict rotary kiln incinerator performance, particularly for intermittently fed containerized waste.

**NUMERICAL MODELS**

Helmrich and Schügerl (1980) present a review of industrial rotary kilns and their characterization. They discuss specific applications of rotary kilns, solids motion and mixing, heat and mass transfer, models including chemical reaction in the bed, and process control. They describe common applications of rotary kilns including the production of lime and cement, the processing of metal ores, and the processing of a wide variety of other minerals. They distinguish between the axial and transverse directions when discussing solids transport, solids mixing, and heat transfer. They describe the motion of solid particles in the various modes of bed motion, particularly slumping and rolling motion, but do not give more than a qualitative description of solids mixing. The discussion of heat transfer to the solids is identical to that of Lehmberg et al. (1977), which assumes intermittent heat penetration into the bed and a gas film resistance between
the bed and the wall. In discussing models of rotary kiln reactors, they list the simplifying assumptions employed by all kiln models then found in the literature. These models are universally one dimensional, assuming complete mixing of gas and solids in the transverse direction, and they always neglect axial mixing and heat transfer in both phases. They describe these lumped parameter models as being generally inadequate in simulating the nonlinear behavior of the real systems, particularly during unsteady state operation. On line computer controls for rotary kiln reactors have met with very limited success because it is very difficult to instrument the process properly and because suitable mathematical models, particularly those describing chemical reactions in the rotary kiln environment, are not available. The authors point out that developing such models and instrumentation would be worthwhile efforts because for many processes there are no reactors capable of replacing rotary kilns, and their main disadvantages in other applications are their inefficiency and temperature control difficulties.

Oran and Boris (1981) present a detailed review of modeling of combustion systems. They introduce the conservation equations for combustion systems and discuss the general problems associated with solving the equations. They cover some of the terms of the equations in more detail and discuss behavior and problems with each type of term. They discuss chemical kinetics, general hydrodynamics, and diffusive transport. The authors present algorithms for dealing with these coupled conservation equations. They cover both supersonic and subsonic reactive flows. Finally, they discuss turbulence and its influence on reactive flows. Detailed modeling is described as being based upon fundamental conservation equations, while empirical modeling is primarily curve fitting of experimental data, and phenomenological modeling is proposing equations that model our intuition of the process. The authors point out that even the best detailed models contain empirical or phenomenological components. They discuss errors that may arise from the approximate nature of the governing equations or the approximate solution
techniques. Without commenting on how well current models work, they point to solution methods and physical models as areas where improvements are needed.

Jones and Whitelaw (1982) focus on calculation methods for turbulent reacting flows. They give the general conservation equations and discuss the numerical methods used to solve these equations. They discuss models of turbulence and combustion and their implications. The authors conclude that the ability of numerical methods to solve turbulent reacting flow problems cannot be described by a general statement. They provide some examples of numerical predictions and experimental data that illustrate this point. They do provide some guidelines for choosing combustion models and solution methods for particular types of problems.

Jenkins and Moles (1981) present a phenomenological model that predicts gas and refractory temperature profiles in a directly fired rotary kiln. The model is designed specifically for a coal-fired rotary cement kiln. The authors use a zonal technique for radiation heat transfer, and they characterize the gas with two gray spectral bands and one clear spectral band. The emissivity of soot and dust in the system is also accounted for with a three band model. The Nusselt number is predicted using an empirical correlation. The authors lack a suitable method for predicting heat release distribution in the flame, so they develop a method to calculate the heat release distribution based upon measured gas concentrations in a field-scale cement kiln. They then predict gas temperatures and wall temperatures and compare them to measured values. The results show relatively good agreement, however the approach seems somewhat impractical as it requires difficult gas concentration measurements to predict temperatures that can be more easily measured.

Clark et al. (1984) present a model for predicting the destruction performance of a pilot-scale liquid injection hazardous waste incinerator having an axisymmetric geometry. The model uses a zone method coupled with a Monte Carlo technique to predict radiant heat transfer. The flow pattern in the system is obtained by actual measurement or by estimation using empirical correlations for specific burner types. A large number of
possible paths through the system are evaluated using a Monte Carlo approach, and a
time/temperature history for each path is calculated. For each path, global kinetics for
waste destruction are applied, giving a fractional decomposition for each path. These
results are then averaged over a large number of paths to get an average destruction
efficiency. The authors claim that the model correctly predicts trends in destruction
efficiency even though it may deviate from measured values by several orders of
magnitude. Due to the poor agreement and the very sparse experimental data, the results
appear inconclusive.

Wolbach and Garman (1984) present a model of chlorinated hydrocarbon
incineration in pilot-scale liquid injection incinerator. In a model which is very similar to
that of Clark et al. (1984), they employ empirical approximations of the flow field and
zonal heat transfer methods to the axisymmetric system. From these, a time-temperature
history for a given path through the system is determined, and simplified kinetic models
are applied to predict the waste destruction. The model is useful for determining the
sensitivity of the system to various operational parameters, and it predicts the temperature
field in the incinerator very well. However, their predicted destruction efficiency for
carbon tetrachloride is two orders of magnitude lower than that measured experimentally.
They conclude that their non-flame mode kinetics model is at fault, and they estimate that
99% of the actual carbon tetrachloride destruction must occur in the flame zone in the real
system.

Gillis and Smith (1988) present a three-dimensional non-reacting flow numerical
model developed to predict flow fields in industrial furnaces. The work is a product of
efforts aimed at modeling pulverized-coal combustion systems. The computer code is
based upon the SIMPLE algorithm (Patankar 1980). Predictions of the complex
isothermal flow field are made for a wall fired furnace using three different turbulence
models, a variety of inlet conditions, and different numerical grid spacings. The model
predictions are compared to experimental measurements obtained during cold flow testing
of a pilot-scale furnace. Predictions using a standard $k-\varepsilon$ turbulence model showed much better agreement with experimental data than did predictions assuming a constant eddy diffusivity or a Prandtl mixing length model. The authors show that important features of the flow are not distinguished if the grid is too coarse. The finest grid used in the study consisted of 102,375 nodes, and the solution remained dependent upon the grid selection. Even considering this difficulty, agreement between the model and experimental data was surprisingly good. Moderate changes in the specified inlet conditions showed relatively large changes in the predicted flow field.

Smith, Sowa, and Hedman (1990) anticipate the ability of comprehensive coal combustion codes to simulate practical systems realistically, and they present a design methodology to minimize the computational cost of the design process. The design strategy is based upon statistical techniques in response surface methodology. The designer selects a design space for the design variables to be adjusted. Response surface methods are used to specify the particular points in the design space that are to be simulated and the numerical model is run with the conditions specified at each point. Statistical regression functions are then used to interpolate between the design points to provide a response surface for each dependent variable. Since the method relies on very few simulation data points, computer time is greatly reduced. A final numerical simulation is performed at the optimum point seen on the response surfaces. If the results of that simulation agree with the response surface predictions, the point is considered the optimum; otherwise a new set of design points is selected in a tighter region of the design space around the preliminary optimum. The authors describe a two-dimensional coal combustion code that includes mixing limited gas phase reaction, coal devolatilization kinetics, and radiation heat transfer. They use this model within the framework of their design methodology to optimize two coal gasifier injector designs for maximum gas production and one coal combustor burner design for minimum NO formation. In all three cases the dependent variable at the optimum was within 1% of the value predicted by
the response surface, demonstrating rapid convergence to the optimum. The authors point out that results obtained using this methodology will only be as good as the comprehensive numerical model, and such models still have much room for improvement.

Numerical models of rotary kilns have been limited to steady-state operation with many simplifying assumptions such as plug flow of the solids and gases. These models tend to consist of one-dimensional differential equations, constituting phenomenological mathematical models. Currently, no detailed numerical model of a rotary kiln incinerator exists in the literature. Detailed numerical models have shown applicability in the study of coal-fired furnaces, although excessive use of computer time and difficulty in validating the predicted results have been obstacles to their use in the design process. Detailed numerical models do show promise for eventually modeling waste incineration in rotary kilns.
February 18, 1992

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CHAPTER 4

FIELD-SCALE ROTARY KILN INCINERATION OF BATCH-LOADED TOLUENE/SORBENT: I. DATA ANALYSIS AND BED MOTION CONSIDERATIONS

INTRODUCTION

The study of hazardous waste incineration in rotary kilns is receiving increased attention, especially as landfill restrictions are expanding to an ever broader range of solid waste materials. Also, as the regulations on hazardous waste incinerators become increasingly stringent, predictive ability for the performance of these systems, even in a rudimentary sense, is needed. Because of the considerable complexity of the process, however, much remains to be learned. As part of our comprehensive study of this process at Louisiana State University, we have recently emphasized the need to broaden the full-scale experimental data base. Such data are needed to provide insight into this complicated process, for use in both model development and validation, and in scaling analyses (Lester et al. 1991). Initially, our field-scale efforts focused on obtaining species and temperatures at the exit of an industrial rotary kiln during quasi-steady processing of liquid carbon tetrachloride (Cundy et al. 1989a, 1989b, 1989c). Subsequent work focused on obtaining continuous gas and temperature measurements during transient processing of polyethylene packs containing clay sorbent charged with toluene (Lester et al. 1990), xylene (Cundy et al. 1991a), and dichloromethane (Cundy, et al. 1991b). These studies were performed on the rotary kiln incinerator operated by the Louisiana Division of The Dow Chemical Company at their facility in Plaquemine, La.
The studies of transient behavior have focused on characterizing the incinerability of an aromatic and a chlorinated hydrocarbon in a rotary kiln environment. Toluene was selected as the aromatic test liquid because it is commonly used as a surrogate waste during trial burns in the permitting process, and because we have used it extensively in bench- and pilot-scale work (Cundy et al. 1989d; Lighty et al. 1989, 1990). Unfortunately, Federal regulations precluded our use of toluene at the Dow facility after the first experiment; thereafter xylene was substituted. Recent facility additions, however, have allowed us to complete our study using toluene. With the experience gained from previous full-scale transient experiments, we have, in this most recent study, been able to perform a much more detailed study of the Dow incinerator system. The experimental variables and conditions have remained largely the same for comparison purposes. The experimental procedures have been improved, and the number of continuous measurements has been greatly increased. The details of this most recent study, including descriptions of the instrumentation and the operating conditions studied as well as some preliminary results, were presented in Chapter 3. Therefore, only a brief summary of the experimental methods will be presented here.

EXPERIMENTAL METHODS

Facility

The Dow rotary kiln incinerator in Plaquemine, La. is 3.2m in diameter and 10.7m long, with a design firing capacity of 17 MW and 800°C outlet temperature. Gases flow through the kiln exit plane, into a transition section, and then into the afterburner. The afterburner has a design firing capacity of 7 MW, a design outlet temperature of 1000°C, and a minimum residence time of 2 seconds. Gases flow from the afterburner through a quench chamber, a series of wet scrubbers and wet electrostatic precipitators, an induced draft fan, and a stack. Figure 4.1 shows a system schematic.
Figure 4.1 Schematic of the Dow rotary kiln incinerator facility showing the measurements taken at each location.

1. Kiln Sampling Probe: O$_2$ concentration
   CO$_2$ concentration
   CO concentration
   THC concentration
   Gas temperature

2. Afterburner Probe: O$_2$ concentration
   CO$_2$ concentration
   CO concentration
   THC concentration
   Gas temperature

3. Stack Sampling: O$_2$ concentration*
   CO concentration (2)*

4. Bed Thermocouple Temperature

5. Kiln Feed End Pressure*

6. Kiln Exit Pressure*

7. Kiln Exit Temperature*

8. Afterburner Temperature*  

* - indicates measurements from instruments that are a permanent part of the facility
Experimental Conditions

Polyethylene packs, each containing 18.9 liters of toluene on 22.7 kg of sorbent (montmorillonite granules of approximately 6 mm diameter), were prepared by Dow personnel before the experiments. Blank packs (sorbent only) were also prepared. One pack was fed into the kiln every 10 minutes throughout the experiment; blank packs were fed while changing operating conditions to maintain bed thickness in the kiln. Two nozzles, located on the stationary kiln face, allow the injection of compressed air (at ambient temperature) into the kiln to promote turbulence, bulk mixing, and combustion; we call this turbulence air. Continuous gas measurements and gas temperatures were obtained during four different test modes: operation with and without the addition of turbulence air and operation at two kiln rotation rates, 0.1 and 0.25 rpm. Table 4.1 gives the experimental test matrix that was used on the two consecutive days of testing.

Table 4.1 Experimental test matrix for each day.

<table>
<thead>
<tr>
<th>No. Packs</th>
<th>Contents</th>
<th>Sampling</th>
<th>Rotation rate*</th>
<th>Turbulence air</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>Blank</td>
<td>None</td>
<td>Fast</td>
<td>Off</td>
</tr>
<tr>
<td>6</td>
<td>Toluene</td>
<td>Continuous</td>
<td>Fast</td>
<td>Off</td>
</tr>
<tr>
<td>3</td>
<td>Blank</td>
<td>None</td>
<td>Fast</td>
<td>Changing</td>
</tr>
<tr>
<td>6</td>
<td>Toluene</td>
<td>Continuous</td>
<td>Fast</td>
<td>On</td>
</tr>
<tr>
<td>3</td>
<td>Blank</td>
<td>None</td>
<td>Changing</td>
<td>On</td>
</tr>
<tr>
<td>6</td>
<td>Toluene</td>
<td>Continuous</td>
<td>Slow</td>
<td>On</td>
</tr>
<tr>
<td>3</td>
<td>Blank</td>
<td>None</td>
<td>Slow</td>
<td>Changing</td>
</tr>
<tr>
<td>6</td>
<td>Toluene</td>
<td>Continuous</td>
<td>Slow</td>
<td>Off</td>
</tr>
<tr>
<td>2</td>
<td>Toluene</td>
<td>Sample bomb</td>
<td>Slow</td>
<td>Off</td>
</tr>
</tbody>
</table>

* Fast - 0.25 rpm, Slow - 0.1 rpm
To the greatest extent possible, all operational parameters were held constant during each test mode. These parameters included: kiln rotation rate, natural gas and air feed rates to the kiln burners, and the turbulence air injection rate. Stack measurements, taken by Dow personnel using EPA approved methods, verified that incinerator emissions remained well within regulatory limits during the entire test period.

**Sampling and Instrumentation**

As in previous studies (Cundy et al. 1989a, 1991a, 1991b), two water-cooled probes were used to obtain gas samples and gas temperature measurements within the kiln and afterburner. Figure 4.1 shows the probe sampling locations and the measurements taken at each location. Each probe is equipped with a radiation-shielded type K thermocouple at its tip. The kiln probe, 7.8 m in length, was inserted through the transition section and drew samples from near the kiln exit. Only two access ports were available; one allowed the probe to reach a point in the upper half of the kiln, while the other allowed the probe to reach a point in the lower half of the kiln. The locations of these two sampling points are shown in Figure 4.2, as calculated using a method detailed by Montestruc (1989). The kiln probe was inserted into the upper access port on the first day of experiments (3 October 1990) and it remained there for the entire day. On the second day (4 October 1990), the probe was inserted into the lower access port and the experiments were replicated. The afterburner probe, 3.8 m in length, was inserted in a different location from previous studies in an effort to sample from a better-mixed region of the afterburner. Sample gases were drawn through each probe using an air-driven jet pump. These gases were cooled by passage through the probe and any condensate was removed using a cyclone separator. The sample gases were next drawn through a Teflon sample tube to a rotary sample pump, then passed through a particulate filter, a chiller, and another condensate trap. The dried sample gas was metered through a flow controller into a series of gas analyzers. All continuous data were recorded using
Omega® data acquisition packages on Macintosh SE® computers, at a frequency of 1 Hz.

A more detailed discussion of the instruments and sample treatment is given in Chapter 3.

Figure 4.2 Location of the two sampling regions near the kiln exit plane. The locations are calculated to within ±0.15 m. This diagram is not drawn to scale.

Along with these measurements, the readings of several Dow facility instruments were continuously recorded during these experiments. Oxygen and CO concentrations in the stack, temperatures in the kiln and afterburner, and pressures in the kiln feed end and transition section were recorded. These locations are also indicated in Figure 4.1.

Measurement of the temperature of the solids bed in the kiln was attempted using a 19 mm diameter heavy wall stainless steel tube supporting a 3.175 mm diameter stainless steel sheathed type K thermocouple. This probe was not cooled and was inserted 1 m into the kiln, where the thermocouple tip was immersed in the bed of solids. Figure 4.1 shows the location of this probe.
The sample gas from the kiln and afterburner probes could also be diverted into one-liter glass sample bottles for later analysis using GC and GC/MS techniques. To simplify the sampling procedure, these grab samples were not taken simultaneously with the continuous measurements. Instead, during the incineration of a single pack at the end of each day, the continuous analyzers were disconnected and a series of grab samples was taken from both the kiln and afterburner probes at predetermined intervals.

Chapter 3 contains the details of this experimental study and the continuous record of the oxygen concentration measured in the kiln, afterburner, and stack. These data show the variation of the transient oxygen concentration as a function of operating condition at different locations within the system. Because the data were for individual packs, differences from pack to pack under the same operating conditions could be observed. These differences were seen to persist through the entire system. Comparison between operating conditions was somewhat obscured by the variation of individual pack responses. Vertical stratification of the oxygen concentration at the kiln exit, however, was readily observed and agreed well with previous transient studies (Cundy et al. 1991a, 1991b). Although the baseline levels of oxygen were affected by the addition of turbulence air to the system, it was unclear if the oxygen response of individual packs was influenced by the turbulence air. Whether kiln rotation rate had any effect on the oxygen response was also unclear.

In this chapter, the data from all monitored channels are considered. The data are averaged over several packs during each experimental condition to reduce the effects of individual pack variations. These averaged data characterize the conditions at each sampling location and demonstrate the influence of the kiln rotation rate and turbulence air addition. In Chapter 5, mass balances will be performed on the data, the evolution rates of toluene will be characterized, and the influence of bed motion on the evolution rates will be discussed.
Data Reduction

For these experiments, the independent variables were kiln rotation rate (0.25 rpm or 0.1 rpm), and turbulence air addition (on or off). An additional variable is the location of the sampling probe near the kiln exit (upper or lower sampling region). For each combination of independent variables, the system was allowed to equilibrate for at least 30 minutes while blank packs containing only sorbent were fed into the kiln. Then a series of 6 toluene charged packs were fed into the system, one every 10 minutes, providing one hour of data at that condition. The experimental test matrix, shown in Table 4.1, was duplicated on two consecutive days with the kiln sampling probe in the upper kiln location on the first day and in the lower kiln location on the second day. All other measurement locations remained the same; therefore, for all measurements other than those from the kiln probe, the experiment was replicated on the second day.

In the unaveraged oxygen data presented in Chapter 3, the effects of the independent variables were difficult to discern from the variation of individual packs. The same is true of the other continuous variables in their unaveraged form. Thus, an average response to a pack during each experimental condition is more useful for comparisons because the variation between individual packs is averaged out while the primary features of the data are retained. Also, since the ultimate goals of this work include performing mass balances and characterizing toluene evolution rates for each experimental condition, the use of averaged data reduces the individual pack variation in these calculations as well.

The procedure for ensemble averaging the data is discussed here and illustrated in Figure 4.3. To generate an average transient response of a given data channel to a single pack, an appropriate time base must first be generated. The time at which each pack dropped into the kiln was recorded during the experiment. This time provides the reference for the transient response of that pack, i.e., for each data point, the time relative to the most recent pack insertion is calculated. Then the ensemble average of the data for each pack at the same relative time is calculated. Figure 4.3 shows examples of the
CO\textsubscript{2} data in the unaveraged form, the relative time based form, and the ensemble averaged form. The ensemble averaging process tends to smooth the data, yielding a result that is easier to compare between experimental conditions.

Figure 4.3 CO\textsubscript{2} data as recorded, in the time based form, and in the averaged form.
For the ensemble averaging process, the 95% confidence intervals about the mean were calculated from the two-tailed Student t statistic as:

\[
\text{Confidence Interval} = \bar{y}_i \pm t_{n-1} \sqrt{\frac{\sum y_i^2 - (\sum y_i)^2}{n(n-1)}}
\]  

\(\bar{y}_i\) = the mean value of the samples at time "i"

\(t_{n-1}\) = the two-tailed student t statistic for \(n-1\) degrees of freedom, \(\alpha=0.025\)

\(y_i\) = the value of a sample at time "i"

\(n\) = the number of samples to be averaged at time "i" (6, one for each pack)

**EXPERIMENTAL RESULTS**

**Averaged Continuous Data**

The averaged data are shown in Figures 4.4 through 4.18. Shown from top to bottom are continuous measurements taken during fast kiln rotation rate with turbulence air off, fast rotation rate with turbulence air on, slow rotation rate with turbulence air on, and slow rotation rate with turbulence air off. In each of these figures, the single vertical axis heading applies to all eight graphs. Figures 4.4 through 4.8 show the \(O_2\), \(CO_2\), gas temperature, \(CO\), and total hydrocarbon data from the kiln. These figures include, on the left hand side (LHS), measurements taken at the upper kiln exit location and, on the right hand side (RHS), measurements taken at the lower kiln exit location.

In Figures 4.9 through 4.18, the graphs on the right show experimental replicates of the data on the left taken one day later. Figures 4.9 through 4.13 show the \(O_2\), \(CO_2\), gas temperature, \(CO\), and total hydrocarbon measurements obtained from the afterburner probe. The \(O_2\) and \(CO\) measured in the stack are given next in Figures 4.14 and 4.15, followed by the bed temperatures, the facility thermocouple temperatures, and the facility pressures in Figures 4.16, 4.17, and 4.18.
Figure 4.4 Oxygen dry mole fraction measured by the kiln probe.
Figure 4.5 Carbon dioxide dry mole fraction measured by the kiln probe.
Figure 4.6 Gas temperature in Celsius measured by the kiln probe.
Figure 4.7 Carbon monoxide dry mole fraction measured by the kiln probe.
Figure 4.8  Total hydrocarbons as methane measured by the kiln probe. PPMV is parts per million by volume.
Figure 4.9 Oxygen dry mole fraction measured by the afterburner probe.
Figure 4.10 Carbon dioxide dry mole fraction measured by the afterburner probe.
Figure 4.11 Gas temperature in Celsius measured by the afterburner probe.
Figure 4.12 Carbon monoxide dry mole fraction measured by the afterburner probe.
Figure 4.13 Total hydrocarbons as methane measured by the afterburner probe. PPMV is parts per million by volume.
Figure 4.14 Oxygen dry mole fraction measured in the stack.
Figure 4.15 Carbon monoxide PPMV measured in the stack. There were two analyzers at this location, and one of the instruments always gave the higher reading.
Figure 4.16 Temperature in Celsius measured by the bed thermocouple probe.
Figure 4.17 Temperatures in Celsius measured by the two facility thermocouples. The higher reading is from the top of the afterburner, the lower reading is from above the kiln exit.
Figure 4.18 Pressures in inches of water measured by the two facility pressure transducers. The higher reading is from the exit end of the kiln, the lower reading is from the burner end of the kiln.
**Kiln O₂ - Figure 4.4**

In the upper kiln (LHS), the magnitude of the oxygen response to the waste containing packs is roughly the same regardless of operating conditions. In the lower kiln (RHS), however, the response is considerably increased when the turbulence air is on. The baseline oxygen values are very low in the upper kiln when the turbulence air is off. The oxygen values are quite high in the lower kiln regardless of operating conditions. The kiln rotation rate, over the range that was studied, appears to have little or no effect on the oxygen responses.

**Kiln CO₂ - Figure 4.5**

The addition of turbulence air lowers the overall levels of CO₂ in the upper kiln (LHS) and increases the magnitude of the CO₂ response in the lower kiln. The levels of CO₂ observed in the lower kiln are substantially lower than those in the upper kiln, particularly with the turbulence air turned off. There is no clearly discernible effect of kiln rotation rate on the measured CO₂ levels in the kiln.

**Kiln Gas Temperature - Figure 4.6**

The addition of turbulence air lowers the overall gas temperature levels in the upper kiln, and increases the magnitude of the temperature response. In the lower kiln, the turbulence air does not clearly change the overall temperature levels, but it does increase the magnitude of the temperature response. The gas temperatures in the upper kiln (LHS) are much higher than those in the lower kiln. The kiln rotation rate appears to have no effect on the kiln gas temperatures.

**Kiln CO - Figure 4.7**

In the upper kiln, relatively large amounts of CO were observed only during operation with turbulence air off. The addition of turbulence air reduced the observed
values to near zero. Very little CO was observed in the lower kiln under any conditions. In the upper kiln with turbulence air off, it appears that the fast rotation rate caused a greater CO response than did the slow rotation rate. However, it should be noted that the CO concentration should be rather sensitive to oxygen levels, and the baseline oxygen level was almost one percent higher during the slow rotation rate conditions. Since the baseline conditions are not a result of the waste combustion and should be independent of rotation rate, this difference in CO response may result from slightly different support flame feed settings.

*Kiln Total Hydrocarbons - Figure 4.8*

Before discussing the total hydrocarbon (THC) data, an operational aspect must be considered. To prevent the loss of hydrocarbons from the sample gas, the THC sample stream was split from the main sample stream before passing through the sample chiller, secondary condensate trap, and desiccant dryers. Unfortunately, excessive condensation in the sample line extinguished the flame ionization detector on a few occasions and greatly reduced the sample flow rate at other times. As a result, the kiln THC data are generally suspect. Note, however, that the instrument appeared to be operating properly during the first set of data obtained in the upper kiln with turbulence air off and fast kiln rotation rate. A substantial THC response was observed in that data, corresponding with high CO levels observed at the same time. For slow rotation rate with turbulence air off in the upper kiln, the THC response is suspiciously flat even though high CO levels were observed. This is probably due to the THC sampling problems mentioned above. All the other operating conditions show low THC levels corresponding to low CO levels. Although this seems reasonable, the sampling problems preclude confirmation of this observation.
In considering the afterburner data and all data presented beyond this point, recall that the two columns of graphs represent experimental replicates obtained on two consecutive days. Only for the data taken with the kiln probe do these columns represent different sampling locations.

**Afterburner O₂ - Figure 4.9**

For the afterburner data, one sees good reproducibility from one day to the next, although the overall oxygen levels are about 1% higher on the second day. On both days, the addition of turbulence air reduced the magnitude of the oxygen response. Since turbulence air addition is accompanied by an increase in overall gas flow rate, while the amount of toluene in the packs remains the same, the effect of pack combustion is diluted by the increased flow. Kiln rotation rate has no apparent effect on the oxygen response.

**Afterburner CO₂ - Figure 4.10**

The reproducibility of the CO₂ data appears very good. Again, the addition of turbulence air appears to dilute the response from a pack. There appears to be little difference resulting from rotation rate.

**Afterburner Gas Temperature - Figure 4.11**

Overall, the afterburner gas temperature response appears to be quite reproducible. It clearly shows the effect of opening the loading chute door for pack insertion into the kiln. This is seen as the sudden drop in temperature at the end of each curve, which results from additional air entering through the kiln loading chute door during pack loading. Sometimes, the temperature level is seen to return momentarily to the baseline value after the door closes but before the pack begins to burn. Notice that the magnitude of the effect due to the loading chute door is reduced when turbulence air is added. This is also true of the peak temperature response due to pack combustion. This is, in both
cases, thought to be due to dilution by the higher gas flow under turbulence air addition. Again, the kiln rotation rate seemed to have no effect on the measured variable.

Afterburner CO - Figure 4.12

The afterburner CO is plotted on the same scale as the kiln CO in Figure 4.7, as this was the approximate range for which it was calibrated. In contrast to the kiln, very little CO is seen in the afterburner under any conditions.

Afterburner Total Hydrocarbons - Figure 4.13

The THC analyzer used with the afterburner probe had the same operational problems as the THC analyzer for the kiln probe. In addition, problems with the sample flow rate caused a very long lag in the instrument response. This is seen in the data taken on the first day, where some small THC spikes occurred approximately 200 seconds after pack insertion. In general, these spikes were not repeated on the second day, so the data should not be considered reliable. However, the overall low levels of THC do correspond to low levels of CO observed in the afterburner on both days.

Stack O2 - Figure 4.14

The stack oxygen response tends to be very smooth, with the minimum occurring later than for kiln or afterburner measurements. The delay may be due to sample flow to the stack oxygen analyzer or to the time required for the combustion gases to flow through the pollution control equipment. In either case, the effects of turbulence air addition and kiln rotation rate are not discernible. One should note that the oxygen levels measured in the stack generally match those measured in the afterburner, indicating little or no air infiltration downstream of the afterburners in the pollution control equipment. Measurements with turbulence air off on the first day are an exception, showing stack oxygen levels approximately 1% higher than those measured in the afterburner.
**Stack CO - Figure 4.15**

In the stack we were able to monitor the two redundant facility CO analyzers, and both are displayed simultaneously in the graphs. For the operating conditions in these experiments, the CO levels in the stack were so low that all we could observe was instrument noise and calibration error. Some increase in the CO level is apparently due to pack combustion; however, it is insignificant compared to the baseline drift and noise. In all the graphs, the same instrument gave the higher readings.

**Kiln Bed Temperature- Figure 4.16**

The kiln bed temperature measurements presented here were measured by a thermocouple probe inserted axially through the kiln's front rotary seal and into the solids bed. Unfortunately, even though the probe consisted of a 19 mm diameter heavy wall stainless steel tube, it was bent substantially during the experiments each day. When one considers the forces acting on the probe due to the drag of the sorbent bed and the occasional pack bumping into it, together with the high temperatures, it is not too surprising that the probe was bent. The data obtained, although somewhat erratic, bears a strong resemblance to the gas temperature data obtained by the kiln probe. The "bed" temperature is seen to drop off before a pack is loaded, as if it were measuring the effect of cold leak air entering from the loading chute door. As a result, we believe that the thermocouple tip was protruding from the solids. This could not be verified visually because a number of steel lid-retaining rings from the plastic packs collected where the end of the probe should have been, as if they were hung on the probe tip. They may have contributed to the bending of the probe. No clear observations can be drawn from these data, except that the temperatures measured with this probe may represent a very rough measure of the bed and kiln wall surface temperatures in this general location.
Two facility thermocouples were monitored during these experiments. One was located near the top of the kiln exit in the transition section, while the other one was located in the afterburner. Under all conditions, the afterburner thermocouple gave the higher reading of the two. One immediately notices the smooth, gentle response of each thermocouple, punctuated by small discontinuities, generally at time zero. The discontinuities are an artifact of the averaging process and show up whenever the continuous data begins or ends. This is caused by the temperature at the beginning of the first pack being slightly different from the temperature at the end of the last pack, causing adjacent averaged values to be slightly different. The same discontinuity presumably occurs in the other ensemble averaged data, but it is such a small effect that it is obscured.

The facility thermocouple responses are very smooth and sinusoidal compared to the gas temperature responses measured by the kiln and afterburner probes. One explanation for this smooth response is that each facility thermocouple is inside a heavy wall 19 mm Monel thermowell, resulting in fairly long thermal time constants. A second explanation is that neither thermowell is radiation shielded. At the temperatures indicated, radiation heat transfer between the refractory walls and the thermowell may be the dominant mode of heat transfer. If this is the case, then the thermocouples are indicating the rise and fall of the refractory surface temperature in the region around the thermocouple. The refractory itself has a long thermal time constant, thus the measured response will be slow and gradual, as was observed. In the afterburner where the temperatures are higher, the refractory to thermowell radiation exchange should be even more dominant. Indeed, the afterburner temperature response is very small in magnitude and it lags the pack insertion considerably more than does the kiln exit temperature response. The temperature measured by the afterburner thermocouple is always substantially lower than the gas temperature measured by the afterburner probe, again consistent with radiation heat exchange with the refractory walls. The temperature
measured by the kiln-exit thermocouple is substantially lower than the gas temperature measured by the kiln probe in the upper kiln exit region. This may be due to the radiatively cool ash quench area below the facility thermocouple acting as a radiant heat sink, or it may be due to a non-homogeneous temperature field at the kiln exit. Overall, the temperatures measured by the facility thermocouples are remarkably repeatable, and the overall temperature levels do not vary in response to the experimental conditions. This is expected because the input air and gas flow rates were set to provide the same temperature for each operating condition.

Facility Pressures - Figure 4.18

The facility pressure transducers at the feed end of the kiln and in the transition section were monitored, and both are presented in the figure. The transition section pressure is always the higher of the two. The data appear noisy compared to the other monitored variables, even though they have been ensemble averaged like all the other data. The responses measured at each end of the kiln by different pressure transducers, even after averaging, show almost exactly the same "noise", to the smallest fluctuation. This would be unlikely if the fluctuations were originating in the instruments, so these rapid pressure fluctuations are evidently present in the kiln and are not instrument noise.

One prominent feature of the pressure response is the dramatic rise before pack insertion associated with air leaking through the loading chute. One may notice that the pressure is somewhat more erratic during the first 100 to 200 seconds after pack insertion. This may be the result of toluene combustion in the kiln. It is important to note that the toluene combustion did not cause a net pressure rise of the sort that could lead to a positive pressure excursion. Finally, since the pressure was a controlled parameter, it shows little variation across operating conditions and is very repeatable.
Gas Chromatographic Data

The gas chromatographic (GC) methods used in these experiments are identical to those used in previous experiments (Cundy et al. 1991b; Morse et al. 1991). The sampling procedure is slightly modified. The gas stream from the sampling probe in the kiln is drawn through a one liter glass sampling bomb with teflon stopcocks. The bomb is purged with the sample gas for approximately 30 seconds, then the stopcocks are closed, isolating the sample. A second sample bomb is then purged and filled, and so on for a total of 6 samples all obtained in series during the combustion of a single pack. The sample bombs are contained in boxes of 3 bombs each, so between the third and fourth samples the lines are disconnected from one box and connected to the next. Samples were taken in the same fashion from the afterburner probe simultaneously with the kiln samples. The continuous monitors were used for the first 6 packs during that operating condition and then were disconnected. The grab samples were taken immediately afterward, during the seventh pack under the same operating condition. Because of time constraints, grab samples were obtained only during slow rotation rate with no turbulence air addition. The samples were obtained at the end of the experiment on both days and were immediately transported to the laboratory and analyzed within several hours.

The results of the GC sample analyses are shown in Figures 4.19 through 4.22. The GC methods quantified N₂, O₂, CO₂, CO, CH₄, C₂H₂, C₂H₄, C₂H₆, C₆H₆, and C₇H₈. The hydrocarbon concentrations measured by the GC were multiplied by the number of carbon atoms in each species and then summed to give a total hydrocarbon measurement in methane equivalents. The GC data are plotted as a function of sample time together with the averaged continuous data obtained on the same day for the same operating condition. In these figures, the 95% confidence intervals are included for the continuous data to show the variability of the continuous data for each pack.
Figure 4.19 GC data (circles) and averaged continuous data (heavy line) obtained from the upper sampling location in the kiln during slow rotation rate and operation without turbulence air addition. The 95% confidence interval on the continuous data is shown by the two light bracketing lines.
Figure 4.20 GC data (circles) and averaged continuous data (heavy line) obtained from the lower sampling location in the kiln during slow rotation rate and operation without turbulence air addition. The 95% confidence interval on the continuous data is shown by the two light bracketing lines.
Figure 4.21 GC data (circles) and averaged continuous data (heavy line) obtained from the afterburner on 3 October 1990 during slow rotation rate and operation without turbulence air addition. The 95% confidence interval on the continuous data is shown by the two light bracketing lines.
Figure 4.22 GC data (circles) and averaged continuous data (heavy line) obtained from the afterburner on 4 October 1990 during slow rotation rate and operation without turbulence air addition. The 95% confidence interval on the continuous data is shown by the two light bracketing lines.
Upper Kiln GC Data- Figure 4.19

The graph of oxygen in the upper kiln shows good agreement between continuous data and the first three GC data points, but poor agreement for the next three data points. The same behavior is seen for the CO\(_2\) data. The questionable GC samples are all from the second box of three sample bombs. It appears likely that an air leak occurred somewhere in the connection of the second sample box, causing the last three samples to be diluted with air. The third graph shows the CO data and again there is very good agreement with the continuous data. The last three data points in this graph apparently show that the CO concentration was very low already, so the effect of sample dilution is not evident. The total hydrocarbon response is shown in the fourth graph. While the continuous THC analyzer showed little or no response, the GC samples clearly show a large response based upon the first three data points. From this we conclude that the kiln THC analyzer was in fact malfunctioning during that operating condition. This means that large amounts of hydrocarbons were present in the upper kiln during both fast and slow kiln rotation rates when the turbulence air was turned off. This corresponds with the high CO levels that were present during these operating conditions. The hydrocarbon species measured in the upper kiln showed that methane was predominant, and no toluene was detected. This is consistent with results obtained during processing of xylene (Cundy et al. 1991a).

Lower Kiln GC Data- Figure 4.20

In the lower kiln, the first three oxygen data points agree fairly well with the continuous O\(_2\) data, although the second data point is below the continuous data. Since the low value is backed up by a correspondingly high CO\(_2\) data point and no likely mechanism exists to cause this type of error in the GC samples, we accept it as a valid measurement. The fourth data point (at 210 seconds) appears to be too high; this sample was probably diluted by an air leak. The last two data points seem unaffected. The CO\(_2\)
data shows reasonable agreement for the first three data points, while the second three
data points are low. We suspect that the second box of three samples had an air leak.
The CO data agree well, all registering low levels. The first three THC data points
indicate a small spike in the hydrocarbon concentration that was not registered by the
continuous THC analyzer. Again one may conclude that this analyzer was not
functioning at that time. The GC analysis showed small quantities of toluene in these
samples, and relatively low concentrations of methane. Again these measurements are
consistent with those obtained during xylene experiments (Cundy et al. 1991a).

Afterburner GC Data on 3 October 1990- Figure 4.21

In the afterburner on the first day of experiments, the $O_2$, $CO_2$, and CO data agree
fairly well, except perhaps the data point at 210 seconds, which could again be
contaminated with an air leak. The THC data show an interesting behavior; the GC
registered elevated levels of hydrocarbons at 30 seconds while the continuous analyzer
registered similar levels at 200 seconds. The continuous analyzer was apparently
operating properly and registering the correct concentrations; however, the sample flow
rate was evidently reduced, causing a three minute delay time before the sample reached
the analyzer. This reduced flow rate could be attributed to the already long sample line
and build up of condensate interfering with the flow controlling rotameter.

Afterburner GC Data on 4 October 1990- Figure 4.22

On the second day of experiments, the afterburner $O_2$ and $CO_2$ data again show
very good agreement. The CO analyzer shows no response due to pack combustion, as
do the GC samples. Both the GC and the continuous THC analyzer indicate low levels of
hydrocarbons and little or no response from pack combustion.

Overall, although there were problems with some of the GC samples and with
sample conditioning for the THC analyzers, the data agreement is generally very good.
The confidence intervals show that the data, particularly the $O_2$ and $CO_2$ responses, were quite repeatable from pack to pack. Considering the difficulties inherent in this type of study in the field, the overall quality of the data is thought to be quite good.

**DISCUSSION OF RESULTS**

This set of experiments was designed to be experimentally similar to earlier experiments that were conducted using packs of xylene and dichloromethane (Cundy et al. 1991a, 1991b). The only major differences were to be the use of toluene and the more extensive instrumentation and data acquisition in the latter experiments. Data taken during the xylene experiments and these toluene experiments should be similar because the two compounds are quite similar in their combustion properties. The stratification between the upper kiln exit and lower kiln exit is seen with both toluene and xylene, as well as during all other experimental studies on this system (Cundy et al. 1989a, 1989b, 1989c, 1989d, 1991a, 1991b). The changes associated with the introduction of turbulence air, particularly the dilution effect and the effect on CO and THC in the upper kiln, were also seen during the xylene experiments.

During the xylene experiments, rotation rate was seen to have a substantial effect on the response to a pack in the kiln. The faster rotation rate was associated with greater magnitude and shorter duration responses for all the measured variables. This effect was totally absent during the toluene experiments. In addition, the xylene experiments often yielded multiple-peaked responses from each pack. The toluene data showed no such tendency for multiple peaks and, in fact, tended to show a very repeatable response characterized by a rapid peak in the measured variable followed by a gradual decay.

Clearly a difference between the toluene and xylene experiments affected the way in which the waste evolved from the sorbent and thus affected the dependence of evolution rate on kiln rotation rate. Observations of the video taken during the experiments have pointed to differences in bed motion as the cause of the difference in
evolution rates. The bed motion during the xylene experiments could be characterized as slumping motion. In this motion regime, solids intermittently tumble down the free surface of the bed, and then follow the wall in a layer below the surface before reemerging to tumble across the surface again. This motion causes the solids to mix, and each part of the bed is repeatedly exposed at the surface. During the toluene experiments, however, the bed exhibited a slipping motion. With this type of motion, the entire bed slips relative to the wall, and it moves as if it were a solid piece, with the same particles remaining on the surface. In this type of bed motion, the solids mix very slowly. The reason for the different bed motions in the two sets of experiments is not entirely clear. The packs were identical except for the type of liquid contaminant added to each, they were fed at the same 10 minute intervals, and the kiln was rotated at the same rates. This should have resulted in the same type of bed motion.

The bed motion is, among other things, dependent upon the roughness of the kiln wall. Since the kiln wall refractory is usually coated with a layer of hardened slag of variable thickness and texture, it is quite possible that the surface was smoother during the toluene experiments, resulting in the slipping motion. Another possible influence is the presence of the bed thermocouple probe during the toluene experiments. Some of the steel lid retaining rings were observed collecting in the area of the probe. If these rings were actually looped over the end of the probe, as we suspect, the probe could have held the conglomeration of barrel pack rings and sorbent together. This would have given the bed some structural integrity, causing it to slip as a whole rather than mixing and slumping. Even the drag of the thermocouple probe alone may have triggered slipping before the bed could rise high enough for a slump to occur.

The presence of slipping motion of the bed during the toluene experiments at first appears unfortunate. Our previous work has led to a scaling model for predicting waste evolution based upon measurements taken in a system of a different size (Lester et al. 1991). The scaling model was lacking in the area of field-scale data; these toluene
experiments were to provide additional field-scale data for use in testing the scaling analysis. Unfortunately, these data cannot be used because the scaling analysis requires similarity of bed motion. There may be a serendipitous side to this story, however. First, the bed motion was most likely influenced by the temperature probe, although unintentionally, even though all other parameters remained the same. This opens up the possibility that the bed motion may be intentionally modified by inserting fixed structures into the bed, allow one to control the bed motion and the resulting mixing and contaminant evolution characteristics. Second, we now have data obtained under similar experimental conditions with similar contaminant species (xylene and toluene), the only difference being the motion exhibited by the bed. This is an opportunity to make comparisons and determine the effects of bed motion on contaminant evolution in more detail. These comparisons will be made in Chapter 5.

SUMMARY AND CONCLUSIONS

A detailed study of unsteady conditions inside the field-scale rotary kiln incinerator operated by the Louisiana Division of The Dow Chemical Company has been successfully accomplished. Experience gained during earlier studies and the use of more extensive instrumentation has provided a clearer picture of the processes occurring within the incinerator and through the entire system. In this chapter, the ensemble averaged data for each monitored variable are presented as a function of experimental conditions. A list of the conclusions that are drawn from this averaged data follows:

- The bed motion during these experiments was observed to be in the slipping regime, in contrast to the slumping bed motion seen in earlier experiments under similar conditions.
• Vertical stratification in the kiln is observed in the \( O_2 \) concentrations, \( CO_2 \) concentrations, and gas temperatures measured there. The upper kiln is characterized by lower \( O_2 \), higher \( CO_2 \), and higher gas temperatures.

• The addition of turbulence air tends to reduce the magnitude of the stratification observed in the kiln.

• Substantial amounts of CO are observed only in the upper kiln and then only during operation with no turbulence air.

• Kiln rotation rate, over the range studied, appears to have no effect on any of the measured variables. This is thought to be a result of the slipping bed motion observed at both rotation rates during these experiments.

• The addition of turbulence air reduces the magnitude of responses to a pack measured in the afterburner and stack, apparently through dilution of the toluene combustion products by the higher gas flow rates.

• Reproducibility of data in the afterburner and stack is quite good. No replicate measurements were taken in the kiln.

• The continuous gas species measurements in the kiln and afterburner agree well with gas chromatographic analyses of grab samples from those locations.
The measured bed temperatures presented here are probably not accurate because of uncertainty in the location of the thermocouple tip; however, they may be a rough measure of the bed and kiln wall surface temperatures.

The temperature responses to pack combustion measured by the facility thermocouples are sinusoidal, and very smooth in contrast to the measured gas temperatures. Large thermowells and lack of radiation shielding on the facility thermocouples appear to explain the discrepancy.

The data presented in this chapter are used to calculate toluene evolution rates and perform mass balances, which are presented in Chapter 5.
CHAPTER 5

FIELD-SCALE ROTARY KILN INCINERATION OF BATCH-LOADED
TOLUENE/SORBENT: II. MASS BALANCES, EVOLUTION RATES,
AND BED MOTION COMPARISONS

INTRODUCTION

An extensive study of an industrial scale rotary kiln incinerator is being conducted by a team of researchers from Louisiana State University and the University of Utah. The focus of the study is a 17 MW rotary kiln incinerator operated by the Louisiana Division of The Dow Chemical Company, in Plaquemine, La. This facility has been described in several previously reported studies (Cundy et al. 1989a, 1989b, 1989c, 1989d, 1991a, 1991b). The experimental details of the current study, as well the entire data set obtained during this study, were presented in Chapters 3 and 4. In these experiments the kiln rotation rate was either 0.1 rpm or 0.25 rpm (slow or fast, respectively), and the kiln was operated with or without the addition of turbulence air (compressed air injected in the front of the kiln to induce mixing and swirl). The four experimental conditions (fast, turbulence air off; fast, turbulence air on; slow, turbulence air on; slow, turbulence air off) were repeated on a second day of testing. During each experimental condition, six plastic packs containing toluene-contaminated clay sorbent were incinerated, one every ten minutes. The transient responses measured throughout the incinerator system for the six packs were ensemble averaged to produce an average response for a single pack under each operating condition. These averaged responses are presented in Chapter 4.
In previous studies (Lester et al. 1991; Cook et al. 1992) continuous gas analyzers were used to monitor conditions only at the kiln exit. Contaminant evolution rates and mass balances were performed using these data, although some very restrictive assumptions were necessary. The primary difficulty was the use of measurements from only two points at the kiln exit to predict the overall species flow rates, even though large gradients in species concentrations and temperature are known to exist there. A system of weighting factors was developed to assign a fraction of the overall flow to the concentrations measured at each probe location. Using these methods, mass balances obtained during operation without turbulence air were quite good. When turbulence air was added to the system, however, the mass balances were not as good.

From the previous work it became clear that measurements taken at the kiln exit, although informative, were not sufficient for calculating contaminant evolution rates and closing mass balances without making gross assumptions. The poor mixedness of the gas stream at the kiln exit does not allow one to calculate accurately the total flow rate of a species without measuring both the species concentration and the gas velocity at numerous locations over the exit cross section. Otherwise, only gross assumptions about the species and flow distribution can be made. The need for better data with which to calculate contaminant evolution rates was one of the motivations for adding continuous measurements of \( \text{O}_2 \) and \( \text{CO}_2 \) in the afterburner and \( \text{O}_2 \) in the stack. The assumption of a well-mixed gas stream characterized by a uniform concentration of each gas species seems much more realistic at these locations. Measurements taken at a single location can then be used to calculate contaminant evolution rates and close mass balances without resorting to complicated weighting factor schemes. Thus, the techniques used in this work are similar to those used in the previous mass balance work, except for the use of different monitored variables and less restrictive assumptions.

In this chapter, the averaged data from Chapter 4 are used, together with metered air and natural gas flow rates, to calculate the average air infiltration rates and the time
dependent toluene evolution rates. Using these results, mass balances are performed and the characteristic times for toluene evolution are determined. The first step in this process is to determine the baseline $O_2$ and $CO_2$ concentrations in the afterburner and the baseline $O_2$ concentration in the stack. These, together with the metered natural gas and air flow rates into the system, are then used to calculate the rate of air leakage into the system. The total air and natural gas flow rates, together with the stoichiometric equation for methane and air combustion, are used to calculate the total flow rate of combustion gas through the system (from the afterburners to the stack). Then, using the combustion stoichiometry of toluene and air, and the deviation of the $O_2$ and $CO_2$ concentrations from baseline, the time resolved toluene combustion rates are calculated. Integrating the toluene combustion rate over time, a mass balance on toluene is performed for the system. Using the cumulative toluene evolution curve, a characteristic time for the evolution process is determined. The toluene evolution rates are compared to the xylene evolution rates obtained by Lester et al. (1991), and the differences, presumably caused by the different types of bed motion, are discussed. Finally, the conclusions of this work are summarized.

**BASELINE FLOW RATE DETERMINATION**

The first step in calculating toluene evolution rates and performing toluene mass balances is to establish the gas flow rates in the system. Incinerator systems operate at a slight vacuum to prevent fugitive emissions; this causes unmetered air infiltration. Because air leakage into the system is not known explicitly, the flow rates must be established from experimental measurements of the baseline combustion products. The term "baseline" refers to the steady conditions existing in the incinerator system without any contaminant or pack combustion. The baseline levels of $CO_2$ and $O_2$ measured in the afterburner and stack are produced only by the natural gas and air introduced into the kiln and afterburner. Even when combustion of toluene perturbs these concentrations, they return to the baseline levels before the next pack is inserted. Figure 5.1 shows a typical
ensemble averaged CO$_2$ trace from the afterburner. The peak in CO$_2$ attributed to toluene combustion is seen, as well as a drop in CO$_2$ mole fraction below baseline shortly before the combustion begins. This drop in CO$_2$ corresponds with the opening of the loading chute door in the kiln to insert the pack, and the resulting inrush of leak air above the baseline flow rate. Although a double door system is used during the loading process, the seal is imperfect. The CO$_2$ mole fraction approaches the baseline level before the loading chute door is opened, and it is seen to resume momentarily the baseline value after the loading chute door closes, but before toluene combustion begins. For this work, the baseline mole fraction of CO$_2$ or O$_2$ is the average of the values exhibited immediately before the loading chute door opens and immediately before pack combustion begins. This value is determined by first graphing the data, drawing a best estimate horizontal line through the data immediately before and after the loading chute door perturbation, and reading the coordinate of this line from the vertical axis in terms of mole fraction. This line and the corresponding value are also shown in Figure 5.1. Although this is a manual procedure, it is the most reliable method available and it is not entirely arbitrary thanks to the presence of the loading chute door perturbation that is used as a marker.

Figure 5.1 Typical averaged CO$_2$ response curve showing important features and baseline. This data was obtained in the afterburner on 3 October 1990 during fast rotation rate, no turbulence air addition.
The following assumptions are made in determining the baseline air leak rate and the total flow rate:

1. The natural gas is assumed to be pure CH₄.
2. The CH₄ undergoes complete combustion with air, providing baseline levels of O₂ and CO₂ against which transients due to toluene combustion can be measured.
3. Combustion of all toluene in a pack is completed before the next pack is inserted 600 seconds later, so that baseline O₂ and CO₂ concentrations may be estimated at the beginning and end of each transient response.
4. No air leakage occurs downstream of the afterburner sampling location.
5. Metered air and natural gas flow rates, together with the calculated air leak rate, yield a total flow rate that is constant under baseline conditions. This assumption is known to be incorrect when the loading chute door is open; however, neither baseline values nor toluene evolution rates are calculated during that period of time.
6. The flow at the afterburner and stack locations is homogeneous with respect to the CO₂ and O₂ concentrations under baseline conditions. Thus, the measured concentrations are representative of the entire flow at these locations.

The following is a derivation of the equations used for calculating the baseline air leak rate and the total flow rate, and the terms are defined in the glossary. The stoichiometry for complete CH₄ combustion with oxygen is given as:

$$\text{CH}_4 + 2\text{O}_2 \rightarrow \text{CO}_2 + 2\text{H}_2\text{O}$$  \hspace{1cm} (5.1)

The combustion process for the kiln and afterburner together, under baseline conditions, may be represented by the following stoichiometric equation:
\[ M_{\text{CH}_4} \text{CH}_4 + (M_{\text{air}} + M_{\text{leak}})(0.208\text{O}_2 + 0.792\text{N}_2) \rightarrow \\
M_{\text{CH}_4} \text{CO}_2 + 2M_{\text{CH}_4} \text{H}_2\text{O} + (M_{\text{air}} + M_{\text{leak}})(0.208\text{O}_2 + 0.792\text{N}_2) - 2M_{\text{CH}_4} \text{O}_2 \] (5.2)

The total molar dry flow rate after the combustion process is obtained from the right hand side of equation (5.2) by summing all coefficients except that for \( \text{H}_2\text{O} \) to yield:

\[ M_{\text{dry flow}} = M_{\text{air}} + M_{\text{leak}} - M_{\text{CH}_4} \] (5.3)

The dry flow rate is of interest because the instruments used to measure the \( \text{CO}_2 \) and \( \text{O}_2 \) concentrations required dry gas samples. From the stoichiometric coefficient for the \( \text{CO}_2 \) produced in equation (5.2), and using equation (5.3) for the total molar flow rate of products, the mole fraction of \( \text{CO}_2 \) in the products on a dry basis is:

\[ [\text{CO}_2] = \frac{M_{\text{CH}_4}}{(M_{\text{air}} + M_{\text{leak}} - M_{\text{CH}_4})} \] (5.4)

Here the bracketed species, \([\text{CO}_2]\), indicates dry mole fraction. Solving equation (5.4) for the air leak rate yields:

\[ M_{\text{leak}} = M_{\text{CH}_4} \left(1 + 1/[\text{CO}_2]\right) - M_{\text{air}} \] (5.5)

An alternative approach for determining the air leak rate is to solve equation (5.2) in terms of the \( \text{O}_2 \) mole fraction on a dry basis. The result is:

\[ [\text{O}_2] = \frac{((M_{\text{air}} + M_{\text{leak}})0.208 - 2M_{\text{CH}_4})}{(M_{\text{air}} + M_{\text{leak}} - M_{\text{CH}_4})} \] (5.6)

Equation (5.6) is then solved for the air leak rate as:
\[ M_{\text{leak}} = M_{\text{CH}_4} \left( 2 - \{\text{O}_2\} \right) / \left( 0.208 - \{\text{O}_2\} \right) - M_{\text{air}} \] (5.7)

Equation (5.5) may be used to calculate the baseline leak rate of air using metered flow rates and the baseline \( \text{CO}_2 \) mole fraction measured at the afterburner. Equation (5.7) will also yield the baseline leak rate of air; it can be applied using either the baseline \( \text{O}_2 \) mole fraction measured in the afterburner or measured in the stack. Regardless of the method used to calculate the leak rate of air, equation (5.3) gives the total dry molar flow rate through the system at either the afterburner sampling location or the stack.

**Table 5.1** shows the metered air and natural gas flow rates, as well as the measured baseline mole fractions of \( \text{CO}_2 \) and \( \text{O}_2 \) at the afterburner and stack, for each operating condition and date. In the table, the experimental conditions are abbreviated, so that the condition of "fast kiln rotation rate with turbulence air off on 3 October 1990" becomes "Fast Off 3". Notice that when the turbulence air is on, the natural gas flow rate is increased, and the metered air flow (which includes both the burner air and the turbulence air) is also increased. This increase in natural gas input is required to heat the added cool turbulence air to maintain the system operating temperature according to the facility thermocouple located at the kiln exit. The values given in **Table 5.1** are those necessary to solve for leak air flow rates using equations (5.5) or (5.7).
Table 5.1 Natural gas and air flow rates, and measured baseline mole fractions of \( \text{O}_2 \) and \( \text{CO}_2 \) as a function of experimental conditions (fast or slow kiln rotation rate, turbulence air on or off, data taken on 3,4 October 1990).

<table>
<thead>
<tr>
<th>Experimental Condition</th>
<th>Natural Gas ( \text{M}_{\text{CH}_4}^* )</th>
<th>Metered Air ( \text{M}_{\text{air}}^* )</th>
<th>( \text{[O}_2\text{]}^{**} ) Afterburner</th>
<th>( \text{[CO}_2\text{]}^{**} ) Afterburner</th>
<th>( \text{[O}_2\text{]}^{**} ) Stack</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fast Off 3</td>
<td>840</td>
<td>4200</td>
<td>0.123</td>
<td>0.050</td>
<td>0.132</td>
</tr>
<tr>
<td>Fast Off 4</td>
<td>870</td>
<td>4480</td>
<td>0.130</td>
<td>0.045</td>
<td>0.127</td>
</tr>
<tr>
<td>Fast On 3</td>
<td>1060</td>
<td>6610</td>
<td>0.133</td>
<td>0.043</td>
<td>0.134</td>
</tr>
<tr>
<td>Fast On 4</td>
<td>1060</td>
<td>7450</td>
<td>0.136</td>
<td>0.044</td>
<td>0.136</td>
</tr>
<tr>
<td>Slow Off 3</td>
<td>870</td>
<td>3920</td>
<td>0.116</td>
<td>0.053</td>
<td>0.127</td>
</tr>
<tr>
<td>Slow Off 4</td>
<td>860</td>
<td>4480</td>
<td>0.125</td>
<td>0.049</td>
<td>0.127</td>
</tr>
<tr>
<td>Slow On 3</td>
<td>1060</td>
<td>6570</td>
<td>0.132</td>
<td>0.039</td>
<td>0.134</td>
</tr>
<tr>
<td>Slow On 4</td>
<td>1050</td>
<td>7450</td>
<td>0.137</td>
<td>0.040</td>
<td>0.135</td>
</tr>
</tbody>
</table>

*Standard cubic meters per hour. To obtain kmol/s, multiply by 1.24E-5.

**Measured baseline mole fraction

The leak air flow rate calculated using each approach, and the resulting total flow rate using each leak rate, are shown in Table 5.2. These total dry flow rate calculations are based upon:

1. leak rate estimated from baseline afterburner \( \text{O}_2 \) mole fraction
2. leak rate estimated from baseline afterburner \( \text{CO}_2 \) mole fraction
3. leak rate estimated from baseline stack \( \text{O}_2 \) mole fraction
4. total flow rate correlated from pressure across the induced draft fan at the stack

Observe that the calculated leak rates are very large; for operation with turbulence air off the leak air flow rate averaged 3.5 times the metered air flow rate, while for operation with turbulence air on the ratio is 2.8. The total dry flow rates calculated from the three leak air flow rates agree rather well; however, the dry flow rate measured across the induced draft fan, even after correction for density and moisture, is generally higher.
Table 5.2 Leak air flow rates and total dry flow rates of combustion products as a function of experimental condition and calculation method.

<table>
<thead>
<tr>
<th>Experimental Condition</th>
<th>Calculated Leak Air Flow $M_{\text{leak}}^*$</th>
<th>Calculated Total Dry Flow $M_{\text{dry flow}}^*$</th>
<th>Measured Dry Flow $M_{\text{dry flow}}^*$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$\text{AB}^1$ $\text{O}_2$</td>
<td>$\text{AB}^2$ $\text{CO}_2$</td>
<td>$\text{Stack}^3$ $\text{O}_2$</td>
</tr>
<tr>
<td>Fast Off 3</td>
<td>14300</td>
<td>13500</td>
<td>16300</td>
</tr>
<tr>
<td>Fast Off 4</td>
<td>16200</td>
<td>15600</td>
<td>15500</td>
</tr>
<tr>
<td>Fast On 3</td>
<td>19600</td>
<td>19200</td>
<td>20000</td>
</tr>
<tr>
<td>Fast On 4</td>
<td>20000</td>
<td>17700</td>
<td>19800</td>
</tr>
<tr>
<td>Slow Off 3</td>
<td>13900</td>
<td>13300</td>
<td>16100</td>
</tr>
<tr>
<td>Slow Off 4</td>
<td>14900</td>
<td>13800</td>
<td>15500</td>
</tr>
<tr>
<td>Slow On 3</td>
<td>19300</td>
<td>21200</td>
<td>19900</td>
</tr>
<tr>
<td>Slow On 4</td>
<td>20300</td>
<td>20000</td>
<td>19500</td>
</tr>
</tbody>
</table>

*Standard cubic meters per hour. To obtain kmol/s, multiply by 1.24E-5.
1) based upon baseline afterburner $\text{O}_2$ mole fraction
2) based upon baseline afterburner $\text{CO}_2$ mole fraction
3) based upon baseline stack $\text{O}_2$ mole fraction
4) total dry flow rate correlated from pressure rise across the induced draft fan

**TOLUENE EVOLUTION RATES**

Once the total flow rates and baseline values for $\text{O}_2$ and $\text{CO}_2$ concentrations have been established, the rate of toluene combustion as a function of time may be calculated. The following additional assumptions are necessary before proceeding:

1. The toluene undergoes complete combustion, forming $\text{CO}_2$ and $\text{H}_2\text{O}$, and consuming $\text{O}_2$. Concentrations of incomplete combustion products such as CO, hydrocarbons, and soot are negligible.

2. The perturbation of the measured $\text{CO}_2$ and $\text{O}_2$ mole fractions caused by combustion of the plastic pack is negligible (Chapter 3).

3. The flow at the afterburner and stack locations remains homogeneous with respect to the $\text{CO}_2$ and $\text{O}_2$ concentrations during the combustion of toluene in the kiln.
4. The combustion of toluene has only a negligibly small effect on the dry gas flow rate at the afterburner and stack. In other words, the flow rates calculated from baseline conditions remain representative during the combustion of toluene (Cook et al. 1992).

5. There is no delay between the evolution of toluene from the sorbent and its subsequent combustion, making the evolution rate of toluene equal to the calculated rate of toluene combustion.

The rate of toluene combustion can be calculated from the measured response of the CO₂ mole fraction in the afterburner or the O₂ mole fraction in the afterburner or the stack. The deviation of the CO₂ or O₂ concentrations from baseline values represents the effect of toluene combustion. The stoichiometry for complete toluene combustion is:

\[ \text{C}_7\text{H}_8 + 9\text{O}_2 \rightarrow 7\text{CO}_2 + 4\text{H}_2\text{O} \]  \hspace{1cm} (5.8)

Thus for every mole of toluene combusted, 7 moles of CO₂ are formed and 9 moles of O₂ are consumed. On the basis of measured CO₂ mole fraction, we can then express the toluene combustion rate (in kmol/s) as:

\[ m_{C_7H_8} = 7([\text{CO}_2] - [\text{CO}_2]_{\text{baseline}}) \frac{\text{M}_{\text{dry flow}}}{3600} \]  \hspace{1cm} (5.9)

Similarly, the toluene combustion rate based upon measured O₂ mole fraction is:

\[ m_{C_7H_8} = 9([\text{O}_2] - [\text{O}_2]_{\text{baseline}}) \frac{\text{M}_{\text{dry flow}}}{3600} \]  \hspace{1cm} (5.10)
Note that since the CO_2 and O_2 concentrations were measured as a function of time, equations (5.9) and (5.10) can be applied to give toluene evolution rates as a function of time.

As seen in Table 5.2, there are four ways to obtain the total dry flow rate (calculation based upon measured afterburner CO_2 mole fraction, calculation based upon measured afterburner O_2 mole fraction, calculation based upon measured stack O_2 mole fraction, and direct measurement from pressure drop across the induced draft fan). Similarly there are three ways to calculate the toluene evolution rate (based upon the mole fraction response of the afterburner CO_2, afterburner O_2, and stack O_2) once the total dry flow rate is specified. This yields 12 possible combinations of flow rate and species response to calculate toluene evolution rate. To reduce the number of combinations, the flow rate and species response methods were grouped in a logical manner. The same data that were used for the total dry flow rate calculation were also used for the toluene evolution rate calculation. Ultimately, four toluene evolution calculation approaches were compared. They are:

1. The dry flow rate, obtained from equation (5.7) using the baseline afterburner O_2 mole fraction, is used in equation (5.10) together with the response of the afterburner O_2 mole fraction to obtain the toluene evolution rate.
2. The dry flow rate calculated using equation (5.5) from the afterburner CO_2 baseline mole fraction is used in equation (5.9) to obtain the toluene evolution rate.
3. The dry flow rate, obtained from equation (5.7) using the baseline stack O_2 mole fraction, is used in equation (5.10) together with the response of the stack O_2 mole fraction to obtain the toluene evolution rate.
The dry flow rate from the induced draft fan measurement is used in equation (5.10) together with the stack O\textsubscript{2} mole fraction response to give a fourth estimate of the toluene evolution rate.

Figure 5.2 shows the resulting toluene evolution rate calculated using method (1) from the CO\textsubscript{2} mole fraction curve shown in Figure 5.1. The toluene evolution rate is normalized by the total amount of toluene initially present in a pack. Notice that the time dependent toluene evolution rate curve is directly related to the CO\textsubscript{2} mole fraction curve. Very similar results are obtained using the O\textsubscript{2} concentrations measured in the afterburner and stack. Since the time dependent toluene evolution rate curves are intermediate results, they are not all shown. However, the toluene evolution curves obtained from the afterburner CO\textsubscript{2} data are presented later in this chapter for comparisons with xylene evolution curves from Lester et al. (1991).

![Normalized toluene evolution rate for fast rotation, no turbulence air addition obtained from afterburner CO\textsubscript{2} response shown in Figure 5.1. The toluene evolution rate is normalized by the total amount of toluene initially present in a pack.](image_url)
TOLUENE MOLE CLOSURE

Once the instantaneous toluene evolution rates are obtained, the calculation of mole balances on toluene is straightforward. One must simply integrate the toluene evolution rates over time to obtain the cumulative toluene evolution. The toluene evolution rate always returns to zero within 600 seconds, so the cumulative toluene evolution should always approach the total moles of toluene initially present in a single pack. The cumulative toluene evolution curves generated from the afterburner CO₂ data and normalized by the total moles of toluene initially present in a pack are shown in Figure 5.3. Similar curves were generated based on the afterburner and stack O₂ responses.

Each toluene-laden pack incinerated in the system contained 0.178 kmol of toluene. The final values of calculated cumulative toluene evolution were normalized, dividing by 0.178 kmol to obtain the closure on toluene. This mole closure is expressed as the ratio of calculated toluene evolution to the toluene content of a single pack. The calculated fractional toluene closures are given in Table 5.3 for each method of calculation and each operating condition. These fractional toluene closures are also shown graphically in Figure 5.4 for each calculation method and operating condition. Overall, the toluene closure is quite good considering the nature of these experiments. Table 5.3 also shows the average toluene closures for each calculation method and experimental condition, and the standard deviation of these values. Based on the data of Table 5.3, the overall average toluene closure is 88% and the overall standard deviation of the data is 18%. The variation of the toluene closure between consecutive days at the same experimental condition is as large as the variation between different calculation methods or between different operating conditions. Thus, there is apparently little influence of the operating conditions on the toluene closure, and the calculation methods
Figure 5.3 Normalized cumulative toluene evolution as a function of experimental conditions. Slow and Fast denote kiln rotation rate, TA on and TA off denote operation with turbulence air on and off respectively. Replicates obtained on 3 October 1990 and 4 October 1990 are shown. The cumulative evolution is normalized by the amount of toluene present in a pack, with 1.0 representing perfect closure.
yield equivalent results. In earlier studies on xylene and dichloromethane using measurements at the kiln exit only (Lester et al. 1991; Cook et al. 1992), closure was not good during operation with turbulence air addition. Since this is not seen in the current calculations, poor closure with turbulence air addition in previous calculations may have occurred because the turbulence air influenced the quality of the assumptions used in the analysis and not because the ultimate evolution of each species was reduced.

Table 5.3 Toluene mass closure fraction obtained for each experimental condition for each calculation method. See also Figure 5.4.

<table>
<thead>
<tr>
<th>Experimental Condition</th>
<th>Toluene Closure</th>
<th>Average</th>
<th>Standard Deviation</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>AB O₂₁</td>
<td>AB CO₂²</td>
<td>Stack O₂³</td>
</tr>
<tr>
<td>Fast Off 3</td>
<td>0.90</td>
<td>1.09</td>
<td>0.76</td>
</tr>
<tr>
<td>Fast Off 4</td>
<td>1.13</td>
<td>1.33</td>
<td>0.84</td>
</tr>
<tr>
<td>Fast On 3</td>
<td>0.97</td>
<td>1.08</td>
<td>0.88</td>
</tr>
<tr>
<td>Fast On 4</td>
<td>0.73</td>
<td>0.79</td>
<td>0.92</td>
</tr>
<tr>
<td>Slow On 3</td>
<td>0.54</td>
<td>0.95</td>
<td>0.78</td>
</tr>
<tr>
<td>Slow On 4</td>
<td>0.57</td>
<td>0.81</td>
<td>0.63</td>
</tr>
<tr>
<td>Slow Off 3</td>
<td>0.80</td>
<td>1.04</td>
<td>0.73</td>
</tr>
<tr>
<td>Slow Off 4</td>
<td>0.79</td>
<td>0.87</td>
<td>0.59</td>
</tr>
<tr>
<td>Average</td>
<td>0.80</td>
<td>0.99</td>
<td>0.77</td>
</tr>
<tr>
<td>Standard Dev.</td>
<td>0.20</td>
<td>0.18</td>
<td>0.12</td>
</tr>
</tbody>
</table>

* average and standard deviation of all 32 values of toluene closure
1) using the afterburner O₂ mole fraction for total flow rate and toluene evolution rate
2) using the afterburner CO₂ mole fraction for total flow rate and toluene evolution rate
3) using the stack O₂ mole fraction for total flow rate and toluene evolution rate
4) using the total dry flow rate measured in the stack together with the stack O₂ mole fraction to get toluene evolution rate
Figure 5.4 Mole closures on toluene as a function of operating condition and calculation method. See also Table 5.3 for the data and explanation of the key.

CHARACTERISTIC EVOLUTION TIME

In previous work (Lester et al. 1991; Cook et al. 1992) the time necessary for the contaminant to evolve was characterized by the evolution interval, defined as the time required for the middle 80% of the ultimate contaminant evolution to occur. This definition was used because the cumulative evolution curves tended to be irregular, particularly near the beginning and end, due to pack breakdown and bed motion effects. From Figure 5.3 one observes that the shape of the cumulative evolution curve for toluene from a slipping bed is very smooth and repeatable for all the data. In fact, the cumulative evolution curves for toluene shown in Figure 5.3 can be closely approximated by an exponential function, with the exponential time constant representing the characteristic time for contaminant evolution. If the cumulative evolution curves of Figure 5.3 are normalized by their final values, yielding $N_{7Hg}(t)$, the resulting curves will begin at 0, approach 1 at the end, and can be readily fit by the expression:
The application of equation (5.11) to fit a typical normalized cumulative evolution curve is shown in Figure 5.5, with a resulting evolution time constant of 120 seconds.

Figure 5.5 Typical cumulative evolution curve, with curve fit through the data over the indicated range and the function containing the fit parameters. The curve fit follows the data extremely closely over much of the range. Data is from the afterburner CO$_2$ response at fast rotation rate with no turbulence air addition on 3 October 1990 (the same data used in Figures 5.1 and 5.2).

Since the data have been normalized and only the time constant is being extracted, the results are only dependent upon the species response used. In other words, differences in the total dry flow rate are normalized out, and there are only three remaining independent normalized evolution rate calculation methods (based upon afterburner O$_2$ response, afterburner CO$_2$ response, and stack O$_2$ response). The cumulative evolution curves obtained from these three methods are fit using equation (5.11), and the resulting
time constants are given in Table 5.4 and shown in Figure 5.6. Table 5.4 also shows the averages and standard deviations of the time constants over the four experimental conditions and over the three calculation methods. The overall average time constant for contaminant evolution is 141 seconds, with a standard deviation of 23 seconds. The time constants appear to be independent of either the kiln rotation rate or turbulence air addition. This is very different from previous studies on xylene and dichloromethane, where both experimental variables were seen to influence the evolution interval. Figure 5.6 also shows that the use of stack O\textsubscript{2}, afterburner O\textsubscript{2}, or afterburner CO\textsubscript{2} in the calculations had no clear effect on the evolution time constant, although the use of afterburner O\textsubscript{2} caused more scatter in the results than did the others.

Table 5.4 Evolution time constants for each experimental condition and calculation method. See also Figure 5.6.

<table>
<thead>
<tr>
<th>Experimental Condition</th>
<th>Time constant (seconds)</th>
<th>Average</th>
<th>Standard Deviation</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>AB O\textsubscript{2}\textsuperscript{1}</td>
<td>AB CO\textsubscript{2}\textsuperscript{2}</td>
<td>Stack O\textsubscript{2}\textsuperscript{3}</td>
</tr>
<tr>
<td>Fast Off 3</td>
<td>137</td>
<td>120</td>
<td>117</td>
</tr>
<tr>
<td>Fast Off 4</td>
<td>141</td>
<td>127</td>
<td>143</td>
</tr>
<tr>
<td>Fast On 3</td>
<td>190</td>
<td>140</td>
<td>155</td>
</tr>
<tr>
<td>Fast On 4</td>
<td>116</td>
<td>103</td>
<td>129</td>
</tr>
<tr>
<td>Slow On 3</td>
<td>95</td>
<td>138</td>
<td>162</td>
</tr>
<tr>
<td>Slow On 4</td>
<td>141</td>
<td>160</td>
<td>153</td>
</tr>
<tr>
<td>Slow Off 3</td>
<td>157</td>
<td>130</td>
<td>128</td>
</tr>
<tr>
<td>Slow Off 4</td>
<td>183</td>
<td>151</td>
<td>158</td>
</tr>
<tr>
<td>Average</td>
<td>145</td>
<td>134</td>
<td>143</td>
</tr>
<tr>
<td>Standard Dev.</td>
<td>32</td>
<td>18</td>
<td>17</td>
</tr>
</tbody>
</table>

* average and standard deviation of all 24 values of the time constant
1) from the afterburner O\textsubscript{2} mole fraction response
2) from the afterburner CO\textsubscript{2} mole fraction response
3) from the stack O\textsubscript{2} mole fraction response
Figure 5.6 Evolution time constants as a function of operating condition and originating data. See also Table 5.4 for data and explanation of the key.

From the comparisons between calculation methods for obtaining toluene closure and evolution time constants, no single calculation method stands out as clearly better than the others. However, the calculation methods are not equivalent in terms of measurement and calculation difficulty. Measurement of the O$_2$ and CO$_2$ concentrations at the afterburner location is far more difficult than at the stack location. Using these measurements to calculate air leak rates is also somewhat troublesome. Furthermore, the total dry flow rate is simply measured at the stack. The simplest method for obtaining toluene evolution rates, therefore, is to use the stack O$_2$ measurements together with flow rates obtained from the induced draft fan at the stack (calculation method 4). Capability for obtaining both of these measurements (stack O$_2$ and stack flow rate) is standard on rotary kiln incinerator facilities since these data are routinely used to certify that the system is operating within permit guidelines. Since the waste evolution rates obtained with these measurements (calculation method 4) are equivalent to those obtained with the other
methods, future evolution rate characterization studies could make use of existing facility instrumentation for waste evolution rate calculations.

EFFECTS OF BED MOTION ON EVOLUTION RATE

As discussed in Chapter 4, the bed of solids was exhibiting slipping motion during the toluene experiments, in contrast to the slumping motion observed previously during the xylene experiments (Lester et al. 1991). This difference in bed motion regime is a result of either the presence of a thermocouple in the solids bed, or a change in the surface roughness of the slag-coated rotary kiln walls. In the slumping motion regime, solids intermittently tumble down the free surface of the bed, and then follow the wall in a layer below the surface before reemerging to tumble across the surface again. This motion causes the solids to mix, and each part of the bed is repeatedly exposed at the surface. During the toluene experiments, the bed exhibited a slipping motion. With this type of motion, the entire bed slips relative to the wall, and it essentially moves as if it were a solid piece, with the same particles remaining on the surface. In the slipping bed motion regime, the solids mix very slowly. The differences in the bed motion regimes preclude the use of this toluene data in the scaling analysis presented by Lester et al. (1991) as was originally intended. It does, however, allow a comparison of evolution characteristics between slipping and slumping beds. Toluene and xylene have similar physical and combustion characteristics, and the experimental conditions were very similar for each contaminant. Since the only major difference between the experiments was the bed motion, comparisons between the xylene and toluene evolution behavior should show the influence of bed motion.

The toluene and xylene evolution rate data are show in Figure 5.7 for the four operating conditions. The normalized toluene evolution rates obtained from the afterburner CO$_2$ are shown. Each graph also contains the normalized xylene evolution rate obtained from ensemble averaged CO$_2$ measurements at the kiln exit using CO$_2$
weighting factors (Lester et al. 1991). All the evolution curves are normalized so that the integral of the curve over time is unity.

The toluene data show good overall repeatability between the duplicate tests at each operating condition, although the magnitude of the initial spike in evolution shows some variation. For all operating conditions, the toluene evolution curves show essentially the same behavior: a quick rise to the maximum followed by a gradual decay back to the baseline. In contrast, the xylene evolution curves show a broader maximum followed by a rapid decline. Also, the xylene data show a marked difference between fast and slow kiln rotation rates, with the slow rotation rate resulting in a much broader, less intense period of evolution. The xylene data for the slow rotation rate show three distinct evolution peaks in each case, with a separation of approximately 80 seconds between the peaks. This separation appears to correspond with the time necessary for a particle to circulate through the bed and return to the surface. None of this behavior is observed in the toluene evolution data.

From the comparisons between evolution for a slipping bed and a slumping bed, some practical observations can be made. First, the evolution behavior observed from the slumping bed is generally better from a kiln operational perspective because of the broader, less intense waste evolution, with less propensity for causing transient "puffs", as defined by Linak et al. (1987a). This difference in evolution behavior may be caused primarily by the action of the hot, clean sorbent material present in the kiln from previous packs. During slumping bed motion, the preexisting bed material repeatedly buries the fresh charge from a new pack. This appears to cause an increased resistance to mass transfer from the buried charge, and possibly reduces the rate of heat transfer to the buried charge as well, resulting in a decline in evolution rate. When the fresh charge is reexposed due to circulation of the bed, the evolution rate increases again. This is in contrast to the slipping bed case, where apparently the fresh charge is never buried by preexisting bed materials but rather lies on top of these materials. For volatile wastes
Figure 5.7 Comparison of normalized evolution rates for slipping bed (Toluene) and slumping bed (Xylene, from Lester et al. (1991)). Slow and Fast denote kiln rotation rate, TA on and TA off denote operation with turbulence air on and off respectively. For toluene, replicates obtained on 3 October 1990 and 4 October 1990 are included.
such as toluene and xylene, the slipping bed motion is much less preferable because it causes higher peak evolution rates that could, if the magnitude is great enough, lead to a transient "puff". However, if the waste is much less volatile or if it is present in low concentrations, a slipping bed motion may be acceptable because rapid evolution of the waste is unlikely. For these wastes, a slipping bed motion may even be advantageous because the contaminated solids do not become buried in the bed, and so could theoretically be cleaned of their hazardous components more rapidly. In Chapter 4 it was observed that the type of bed motion exhibited may be controllable by the drag exerted by stationary protuberances extending into the bed, or by controlling the roughness of the kiln's inner walls. More extensive work is needed to characterize better the controllability of bed motion and its effects on a variety of waste materials in field-scale incinerators.

SUMMARY AND CONCLUSIONS

In this study, a field-scale rotary kiln incinerator is used to obtain data on the processing of toluene contaminated sorbent contained in plastic packs. The incinerator is probed in several different locations with instruments that continuously monitor species concentrations, temperatures, and pressures. Visual observations indicate that the bed exhibited slipping motion during these experiments. Evolution rates for toluene are determined from experimental data, and cumulative evolution curves are generated. These cumulative evolution curves are very nearly approximated by an exponential function, and as such can be characterized by an exponential time constant. The time constants for toluene evolution average 141 seconds and are not dependent upon either kiln rotation rate or turbulence air addition. Air leak rates into the system are calculated to be between 2.8 and 3.5 times the metered air flow rates. Mass balances on the toluene are performed, yielding good results that are also independent of experimental conditions. Evolution time constants and toluene closure calculations were comparable regardless of the calculation method used. This suggests that stack oxygen concentrations and stack flow rates may be
the preferred data for these purposes because they are monitored in existing rotary kiln incinerator facilities.

Comparisons with evolution data taken previously suggest that the slipping bed motion exhibited during these toluene tests caused the toluene evolution rate to be independent of kiln rotation rate. The slumping motion exhibited during earlier xylene tests apparently restricted mass transfer thus causing the xylene evolution to occur over a longer time with lower peak evolution rates. From an operational perspective, the slumping motion may be preferable for high concentration volatile wastes because it results in a more steady waste evolution. However, for low volatility wastes or low concentration wastes, the slipping bed motion may be advantageous by reducing the mass transfer resistance thus reducing the time to remove the waste from the solids. More work needs to be done to address these possibilities.

NOMENCLATURE

\( \text{CH}_4, \text{O}_2, \text{CO}_2, \text{H}_2\text{O}, \text{C}_7\text{H}_8 = \) methane, oxygen, carbon dioxide, water, and toluene species, respectively, used in stoichiometric equations.

\( [\text{O}_2], [\text{CO}_2] = \) measured mole fraction of oxygen and carbon dioxide on a dry basis as a function of time.

\( [\text{O}_2]_{\text{baseline}}, [\text{CO}_2]_{\text{baseline}} = \) measured mole fraction of oxygen and carbon dioxide on a dry basis under baseline conditions (no waste combustion).

\( M_{\text{CH}_4} = \) metered molar flow rate of methane into the kiln and afterburner. (kmol/s)

\( M_{\text{air}} = \) metered molar flow rate of air into the kiln and afterburner. (kmol/s)

\( M_{\text{leak}} = \) molar flow rate of air leaking into the kiln and afterburner. (kmol/s)

\( M_{\text{dry flow}} = \) total molar flow rate of all product species except water. (kmol/s)

\( M_{\text{C}_7\text{H}_8} = \) molar flow rate of toluene evolution from the sorbent. (kmol/s)

\( N_{\text{C}_7\text{H}_8}(t) = \) molar evolution rate of toluene at time \( t \), normalized by 0.178 kmol. (1/s)
CHAPTER 6

A 3-DIMENSIONAL DETAILED NUMERICAL MODEL OF A FIELD-SCALE ROTARY KILN INCINERATOR

INTRODUCTION

Although rotary kiln incinerators are routinely used in the treatment of solid hazardous wastes, the complex transport and chemical processes occurring within these systems are still not well understood. These processes include gas-phase and flame-mode chemical reactions, surface desorption kinetics, heat transfer including conduction, convection, and radiation, solids mixing and bed motion, mass transfer in porous materials, turbulent heat and mass transfer in the gas phase, thermal buoyancy, and flow in a complex geometry. Ultimately, the combined effects of these processes yield a stream of gas that often requires further processed by an afterburner to destroy any remaining hazardous organic species, and an ash stream that must be sufficiently clean for landfilling. Rotary kiln incinerators are required to operate within an envelope of permit conditions to ensure that the exhaust streams are sufficiently clean. Normally these systems are overdesigned and operate well below the regulatory emission limits, but at a cost in capital and fuel. If the processes governing the destruction of waste within the kiln can be well characterized and modeled, then improvements in the performance and economics of new and existing rotary kiln incinerators may be realized.

The majority of studies performed on rotary kiln incinerators have focused on measurements taken at the stack, where sampling is relatively straightforward. These studies have been helpful in measuring the overall performance of the incinerator
system, but they provide little insight into the details of the processes occurring within the rotary kiln. A number of experimental studies have focused on elucidating the complicated processes occurring within rotary kiln incinerators (Cundy et al. 1989a, 1989b, 1989c; Chapters 3, 4, 5). The measurements presented in Chapters 3, 4, and 5 were obtained by inserting large water cooled probes into the exit regions of an operating industrial rotary kiln incinerator. Unfortunately, difficulties in obtaining experimental measurements in the inaccessible interiors of these systems have left large gaps in our understanding. The geometry of a rotary kiln, with its large, rotating steel drum, makes access for experimental measurements within the system very difficult. The high temperature, corrosive, particulate laden process gases add further difficulty to sampling and measurement.

The observations by Cundy et al. and those in Chapters 3-5 have yielded useful insights into the processes occurring in rotary kiln incinerators. They repeatedly observed a high degree of stratification in temperature and species at the kiln exit, and postulated that it was due to buoyancy of hot gases in the system. This stratification could have a major impact upon waste destruction in the system, but a clearer understanding of the process is needed. Measurements of the temperature, species, and flow field throughout the rotary kiln could provide better understanding, but only the exit region of the kiln is currently accessible to measurement.

A few attempts at modeling rotary kilns and incinerators have been made. Jenkins and Moles (1981) present a phenomenological model of heat transfer in a rotary kiln. This model uses empirical flow field predictions together with zonal heat transfer methods, but relies upon experimental data to supply flame heat release within each zone. Clark et al. (1984) and Wolbach and Garman (1984) present models of chlorinated hydrocarbon incineration in pilot-scale liquid injection incinerators. Both groups employ empirical models of the flow field, zonal heat transfer models, and simplified kinetic models to predict the waste destruction. Others, such as Williams et
al. (1988), have resorted to experimental measurements of cold flow in scale models to predict rotary kiln and afterburner flow fields.

These modeling efforts have yielded some useful information about both incinerator performance and the ability of empirical models to predict performance. Because these models attempt to use a very limited understanding of the processes occurring within the system to make simplifying assumptions, they fall short in their predictive ability. Better success has been obtained recently in the area of coal fired furnaces, where extensive experimental studies have yielded a good overall understanding of the physical and chemical processes involved, and suitable numerical models have been developed. These detailed numerical models of coal fired furnaces have reached the stage where they are useful for predicting the performance of systems in the design process, as discussed by Smith et al. (1990).

In this chapter, a 3-dimensional detailed numerical model of a field-scale rotary kiln incinerator is presented. The purpose of this model is not to predict the performance of a rotary kiln incinerator; instead, the intent is to help elucidate the temperature and flow field that exist within the rotary kiln. An additional goal is to clarify how buoyancy and other operational parameters influence the temperature and flow field. Results are presented for two baseline cases with only the support burners firing the kiln and no waste combustion occurring. These results are compared with the experimental data of Chapters 4 and 5 to verify that the model predictions are physically realistic. No attempt is made to adjust the model to improve its agreement with the experimental data. A parametric study is then performed to determine the effects of buoyancy and several operational parameters on the temperature and flow field. Results obtained for each of these cases are compared and contrasted with the baseline cases. Because the model is intended to predict gross features and parametric trends, useful results are obtained even though some simplifications and approximations are used in
defining the numerical problem. Overall conclusions are drawn, and possibilities for future numerical work in this area are discussed.

**PHYSICAL SYSTEM TO BE MODELED**

This model focuses on an industrial-scale rotary kiln incinerator that is described in detail by Cundy et al. (1989a) and Montestrucl (1989). The rotary kiln is 10.7 meters long and 3.15 meters in internal diameter. The feed end of the kiln is shown schematically in Figure 6.1, as viewed from within the kiln. The loading chute opening, located in the lower center of the kiln face, is where solids are normally fed into the kiln. The support burners are located off the center axis to the right of the loading chute. The upper and lower burners feed a sub-stoichiometric mixture of air and natural gas, while the central burner is normally used for feeding waste oil or solvents. All three burners are angled so that their axes converge on the center axis of the kiln at a point 6.17 meters from the feed end. An opening for sludge feed is located to the left of the loading chute. Normally, steam is fed through the sludge nozzle for cooling when sludge is not being fed. Two other nozzles are located in the upper left and lower right of the kiln face for injecting air. The primary purpose of this air injection is to induce gas phase mixing, but it also adds air to support combustion. These air nozzles inject streams of air in the indicated off axis directions; this air is henceforth referred to as turbulence air (TA). The gas from the burners, nozzles, and air leaks flows through the kiln and exits the kiln into a transition section where it is turned to flow upward into the afterburners. Ash and solids fall from the kiln exit into a sump where they are quenched in water. This is shown in Figure 6.2.
Figure 6.1 Schematic of the rotary kiln feed end as viewed from within the kiln.

Figure 6.2 Schematic of the rotary kiln and transition section in a vertical plane along the direction of flow. Drawing is not to scale.
It must be pointed out that the region of interest in this model is the area inside of the rotary kiln, especially near its exit where measurements have been made. A transition section is included in the computational domain on both physical and numerical grounds. If the kiln were modeled alone with gases exiting the round opening in the horizontal direction, buoyancy would cause an inward flow through the lower part of the outlet plane. This reverse flow, unspecified in the model, would lead to unrealistic results or preclude convergence. In the transition section, the outlet plane is at the top of the computational domain, above and perpendicular to the kiln exit. The hot gas within the kiln flows axially until it reaches the transition section, where it turns and flows upward toward the exit. The transition section acts like a chimney, ensuring outward flow through the exit of the computational domain. This also allows a zone of recirculating flow to reside in the kiln exit plane without violating the outward flow exit boundary condition of the numerical model.

The kiln rotates slowly during operation: the rotation rates studied in Chapters 3-5 are 0.25 and 0.1 rpm. At the higher rotation rate, the velocity of the inner surface of the kiln is only 0.042 m/s. This velocity is so small relative to the gas velocities that its influence on the flow field is negligible. Therefore, in this model the walls are assumed to be stationary.

The kiln operates at a very slight vacuum relative to the atmosphere. This prevents hazardous species from leaking out of the system but it allows substantial quantities of air to leak into the system. Montestruc (1989) estimated that this leak air was between 1.5 and 2.1 times the metered combustion air flow rate into the system, including the afterburners. In Chapter 5, the leak was calculated to be between 2.8 and 3.5 times the metered air flow. Air is known to leak into the kiln around the double doors of the loading chute, and through the rotary seals at both ends of the kiln. Additional air is thought to enter in the transition section although the exact location is unknown. Unfortunately, the flow rate of leak air at each point of entry is not known.
MODEL FORMULATION

Model Inputs

This particular rotary kiln incinerator has been the subject of an extensive experimental study (Chapters 3-5), and substantial amounts of experimental data as well as input flow rates and operating conditions have been recorded. These data provide most of the needed boundary conditions for a numerical model; however, some variables such as leak air flow rate and location are more difficult to quantify. These unmeasured input variables are estimated based upon the best available information, and the details of this process follow.

The metered air, gas, and steam flow rates through each inlet into the kiln were recorded during a detailed set of experiments (Chapters 3-5). During these experiments, natural gas was fed through only two of the support burners; the middle burner received only air. The natural gas was assumed to be pure methane, and the temperatures of the air and gas were assumed to be the ambient temperature during the experiments, at 306 K. In the burner nozzles receiving natural gas, steam was also injected, and an enthalpy balance was used to determine the temperature of the input stream. These input values are provided in Chapter 5 for the baseline cases with and without turbulence air added. It is important to note that during the experiments, when turbulence air was turned on, the natural gas flow rates to the support burners were increased substantially while the air flow rates to the support burners remained the same. The overall combustion stoichiometry in the kiln, including the leak air, remained the same in either case, but the support burners themselves were substantially more fuel rich during TA-on operation (Chapter 5).

The determination of leak air flow rates was more problematic. Although the total amount of un-metered air entering the system was determined for each baseline case, the flow rate at each point of entry was unknown. Although the loading chute is
blocked by two steel doors, there are gaps around the doors where air can enter. Of the total calculated leak flow rate, 35% is assumed to enter at this location. Because the overall opening is rather large and the door is recessed from the kiln face, little heating of the leak air should occur; therefore, the inlet temperature is estimated to be slightly above ambient, at 310K. These values are best estimates; unfortunately, more detailed measurements are not feasible at this time.

The rotary seals on each end of the kiln are known to have small passages where air can leak into the kiln. Although the passages are small, the seals are large, occupying the perimeter of the kiln. Because of this, the total amount of air leaked through each seal is not negligible and each is assumed to contribute 20% of the total leak rate (40% for both seals together). Because the air enters through small passages in the relatively hot seals, some heating should occur. The air entering the seals is therefore assumed to be at 400K.

This leaves 25% of the leak air to enter through leaks in the transition section. The actual sources of the leak might be the view ports or the bottom of the ash quench sump. Because any ambient air leaking into this region will be colder and denser than the hot gas inside, it will probably sink to the bottom of the sump. As it slowly warms and mixes, it will rise, being displaced by fresh leak air. To simplify this complicated and speculative flow, the remaining 25% of the leak air is assumed to rise from the bottom of the ash sump in a uniform fashion. Its inlet temperature is assumed to be 310K.

The walls of the rotary kiln, as well as the kiln face and the transition section walls, are lined with refractory brick. The actual temperatures of these walls are not known so they must be estimated. The refractory brick is thick for the purpose of reducing heat losses through the walls, and therefore could be assumed adiabatic. However, because of the extremes in gas temperature in this kiln and the regenerative nature of heat transfer in rotary kilns (Gorog et al. 1982), the walls are better treated as
isothermal. Based upon the temperatures measured by the facility thermocouple at the kiln exit and other thermocouples in the system (Chapter 4), the kiln walls and face are assumed to be at 800K. Because the transition section contains relatively cool air as measured by Cundy et al. (1989), its wall temperature is assumed to be 400K.

Admittedly, establishing the leak air flow rates, leak air temperatures, and wall temperatures involves considerable estimation. However, this is considered a better option than ignoring the existence of leak air or assuming adiabatic walls simply because detailed information is lacking. We certainly feel that the considerable expertise we have gained with this system justifies the use of best-guessed values when better data are unavailable. All the estimates are based upon some physical evidence, often visual observations. Because one of the goals of this model is to help understand how buoyancy and leak air influence the kiln flow field, a parametric study should meet this goal even if the input values are not exactly correct.

Model Details

A commercially available finite difference code, FLUENT V3.03, was supplied under an academic license by Creare.x Inc. and was used in this work. The code is flexible in allowing the user to apply a variety of solution algorithms, differencing schemes, and sub-models of specific phenomena to a particular problem (Creare.x 1990). The problem is specified using a menu driven interface, and no programming is necessary. For this work the code was run on a dedicated 33 MHz 486 personal computer.

In order to model the incinerator, the continuity and momentum conservation equations must be solved. The coupled equations are solved using the Semi-Implicit Method For Pressure Linked Equations-Consistent or SIMPLEC algorithm (Van Doormal and Raithby 1984). Because the flow is turbulent, a two (differential) equation turbulence model is used to predict the kinetic energy of turbulence ($\kappa$) and its
dissipation rate ($\varepsilon$). The Algebraic Stress Model (Creare.x 1990) then uses these to solve algebraic approximations of the differential transport equations for the Reynolds stresses. In contrast with the standard $\kappa - \varepsilon$ model that uses the Bousinesque hypothesis to incorporate an effective turbulent viscosity, the Algebraic Stress Model is more general, particularly for the swirling flows which occur in parts of the incinerator, and it does not require the assumption of isotropic turbulence. The conservation equations are discretized using the quadratic upwind scheme, known as QUICK (Creare.x 1990), to improve the accuracy of the model in regions where the flow direction is not along the coordinate axes. This also tends to stabilize the model, allowing it to converge more easily.

The energy equation is solved in terms of enthalpy, and the temperature is then extracted from the result. Radiation heat transfer is not included in this model because it adds substantially to the complexity of the problem, and the necessary input parameters for radiation heat transfer in this system are not well known. Although this is a severe simplification, it is deemed necessary at this time to obtain a manageable formulation that will converge. The species conservation equations are solved, and the species of interest in this problem are $\text{N}_2$, $\text{O}_2$, $\text{CH}_4$, $\text{CO}_2$, and $\text{H}_2\text{O}$. Mixing limited methane combustion kinetics are implemented using the model of Magnussen and Hjertager (1977). Because the problem focuses on stratification of the flow, a gravitational acceleration vector is included in the momentum equations, and the density of the gas is calculated as a function of temperature and composition using the ideal gas model.

Although the fluid viscosity is dominated by the effective turbulent viscosity, the laminar viscosity is also specified. The laminar viscosity for air is used, and a fourth order polynomial fit of the temperature variation is used between 300K and 3000K. The data were obtained from Incropera and DeWitt (1985). Similarly, the laminar thermal conductivity is approximated by a fourth order polynomial for air over the same temperature range using data from the same source. The enthalpy of the gas is specified
by integrating the specific heat capacity from a reference temperature to the actual temperature. The composition of the gas is accounted for by computing the mixture specific heat capacity as a mass fraction weighted average of the individual pure component heat capacities. The heat capacities of the pure components are specified as second order polynomials in temperature, and were obtained from Theodore and Reynolds (1987).

Although the kiln itself is cylindrical, a rectangular coordinate system is used to grid the computational domain in this model. This is done because the location and flow area of the off-center burners, as well as the loading chute door and the rectangular transition section, are more readily matched in the rectangular grid. This requires the cylindrical walls of the kiln to be approximated roughly as shown in Figure 6.3. Although this is not physically realistic, the error associated with the stepwise curved wall is unimportant relative to that caused by the coarse nature of the grid itself. The computational grid on a vertical slice along the long axis of the kiln is also shown in Figure 6.3, as well as the coordinate system that will be referred to throughout this chapter. The grid is uniform in each of the three coordinate directions and consists of a total of 12,240 control volumes, of which 9,180 are interior control volumes. Each interior control volume's dimensions are 0.21 by 0.21 by 0.38 m in the X, Y, and Z directions respectively. A complete listing of the model specification, including the grid node locations, all boundary conditions and velocities, the specified properties, and the variables solved is included in Appendix A.
Figure 6.3 Computational grid and coordinate system used in the model a) at the burner end of the rotary kiln (Z=0), b) along the axis of the rotary kiln (X=8). The drawings are not to scale.
Convergence

To solve the specified numerical problem, attention must be given to preventing divergence. First, appropriate relaxation factors are selected. These are shown for each solved variable in Table 6.1. To aid convergence further, multiple sweeps were used for each variable, and these are also shown in Table 6.1. These sweeps represent consecutive iterations solving only that variable without updating the coefficients used in the equations. By using more sweeps for each variable, particularly for the pressure and enthalpy, the intermediate solutions for the variables better satisfy the governing equations before updating the coefficients and beginning another overall iteration through all the variables. This causes the overall iterations to require more processing time, but it helps to stabilize the solution and leads to better convergence.

Table 6.1 Solution parameters for each solved variable.

<table>
<thead>
<tr>
<th>Variable</th>
<th>Number of Sweeps</th>
<th>Relaxation Factor</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pressure</td>
<td>30</td>
<td>0.6</td>
</tr>
<tr>
<td>X-Velocity</td>
<td>8</td>
<td>0.3</td>
</tr>
<tr>
<td>Y-Velocity</td>
<td>8</td>
<td>0.3</td>
</tr>
<tr>
<td>Z-Velocity</td>
<td>8</td>
<td>0.3</td>
</tr>
<tr>
<td>Turbulence K.E.</td>
<td>8</td>
<td>0.3</td>
</tr>
<tr>
<td>T.K.E. Dissipation</td>
<td>8</td>
<td>0.3</td>
</tr>
<tr>
<td>Enthalpy</td>
<td>30</td>
<td>0.6</td>
</tr>
<tr>
<td>N&lt;sub&gt;2&lt;/sub&gt;</td>
<td>2</td>
<td>0.6</td>
</tr>
<tr>
<td>O&lt;sub&gt;2&lt;/sub&gt;</td>
<td>8</td>
<td>0.6</td>
</tr>
<tr>
<td>CH&lt;sub&gt;4&lt;/sub&gt;</td>
<td>8</td>
<td>0.6</td>
</tr>
<tr>
<td>CO&lt;sub&gt;2&lt;/sub&gt;</td>
<td>8</td>
<td>0.6</td>
</tr>
<tr>
<td>H&lt;sub&gt;2&lt;/sub&gt;O</td>
<td>8</td>
<td>0.6</td>
</tr>
</tbody>
</table>

In this work, convergence is judged using two criteria. First, if the values of the variables are not changing significantly over many iterations, the solution is converged. This can be observed qualitatively overall, and quantitatively for a selected number of
variables at specific locations, but it is impractical to quantify overall. To quantify the degree of convergence overall, the normalized residual sum for each variable is used. A residual is the amount that a variable at a particular node must change to satisfy the current discretized equation for that location. These residuals are normalized by the value of the variable to give a dimensionless fraction, and these are summed over all the computational nodes to give the normalized residual sum for that variable. For a better converged solution, these normalized residual sums become smaller for all the variables.

To simplify comparisons of relative convergence for similar models, these normalized residuals sums can be summed over all the calculated variables to provide a single overall sum of normalized residuals. This overall sum of normalized residuals was less than 0.009 in every model solution, including the parametric study cases.

Initial attempts to obtain converged solutions to the kiln model were only partially successful. Often, as a solution was converging smoothly, sudden divergence would occur. Sometimes the solution would stop improving for thousands of iterations even though the residuals were not small. These difficulties are not unusual for complex, three dimensional furnace models where the fluid dynamics, heat transfer, and chemical reactions are strongly coupled. To provide more control over the convergence process, the model was formulated as a transient problem with steady boundary conditions. The problem is solved by obtaining a partially converged solution at a given point in time, then using this as the initial condition to solve the same problem a small time increment later. If the time step is small enough, the initial conditions are a good estimate for the solution after the time step, and only small changes in the variables are made. After a sufficient number of time steps, a steady solution can be reached if the boundary conditions are not changed. This approach is similar to under-relaxation but it tends to provide better stability although it also tends to require more computational time. Furthermore, it tends to localize the influence of conditions at one node on the variables elsewhere in the system. This is intuitive; a parcel of gas cannot move very far
in a short period of time. This also allows better convergence to be obtained at the intermediate time steps than could be obtained if the problem were cast in a steady state formulation. For each step in time, 20 overall iterations were performed, again to obtain better converged intermediate results and stabilize the solution process.

**BASELINE MODEL RESULTS**

**TA-off Results**

The baseline case for the kiln model was solved first for TA-off conditions and the results were used to paint a qualitative picture of the temperature, species, and flow fields within the kiln. Again, the baseline case used gas and air flow rates to the burners that matched those during the experimental tests (Chapters 3-5). Leak air flow rates calculated from the experimental data were included at the loading chute door, the front and rear seals, and the ash sump in the transition section.

The vector components of the velocity at four different vertical slices parallel to the kiln axis are shown in Figure 6.4. High velocities originate at the two burners in use, and these jets rapidly turn upward and coalesce (see the X=13 plane). The jet reaches the top of the kiln about 3 meters from the kiln face, and it then accelerates toward the kiln exit. After passing through the kiln exit plane, the jet turns and flows upward toward the outlet boundary. A recirculation zone exists in the top front of the kiln, above the loading chute door. In the centerline slice (X=8), cold leak air entering through the loading chute is seen to drop to the kiln floor and flow toward the exit. About 6 m from the burner face, this leak flow merges with another flow originating at the kiln exit. The two flows then rise and become entrained in the high speed jet near the top of the kiln. The reverse flow at the bottom of the kiln exit plane appears to be driven by the buoyancy of the warming gases in the center of the kiln floor, and their subsequent entrainment in the low pressure jet in the top of the kiln.
Figure 6.4 Vector velocity component plots for TA-off operation. These plots are vertical slices parallel to the center axis of the kiln (see Figure 6.3).

Scale: Maximum velocity vector shown is 10.7 m/s
Figure 6.5 shows the temperature field at six slices across the kiln axis. The figures show a nearly homogeneous temperature in the recirculation zone against the burner face of the kiln (Z=1). The cool air entering the loading chute door is clearly visible below this recirculation zone. Progressing down the kiln axis (increasing Z), a high temperature flame zone forms and quickly rises to the top of the kiln. This high temperature zone corresponds to the high velocity flow in the top of the kiln. The temperature field becomes highly stratified, and this persists through the kiln exit.

Model Verification-Comparison with Experimental Data

In order to determine if the model predictions are physically realistic, they are compared to the limited experimental data available. During the experimental studies with this rotary kiln incinerator (Chapters 3-5), measurements were taken at two locations near the kiln exit. A diagram showing these sampling points is given in Figure 6.6. Measurements taken at these locations included gas temperature, dry O$_2$ mole fraction, and dry CO$_2$ mole fraction. Measurements of CO and total hydrocarbons were also taken, but their measured values were very low under baseline conditions, and the complete combustion reactions used in this model do not allow for their prediction. Measurements were taken at each location during operation with kiln rotation rates of 0.25 rpm (hereafter termed "fast"), and 0.1 rpm (hereafter termed "slow"). Table 6.2 shows the average experimental data during these operating conditions and the corresponding values predicted by the model, and Figure 6.7 shows bar charts of the same data. Figure 6.7 shows that kiln rotation rate had little effect on the measured values, but location in the kiln strongly influenced the data. The model predictions and experimental data show the same trend due to location: high O$_2$, low CO$_2$, and low temperature in the lower kiln, and low O$_2$, high CO$_2$, and high temperature in the upper kiln. This trend has been observed experimentally in a number of studies with this
Figure 6.5 Gas temperature plots for TA-off operation. These plots are slices across the kiln axis at the specified axial locations (see Figure 6.3).
Figure 6.6 Experimental sampling locations in the numerical reference frame. The axial location is in the $Z=25$ plane (see Figure 6.3), 1.2 m from the kiln exit plane. The burners and loading chute door outlines are added only for perspective.

Table 6.2 Comparison of model predictions with measured data for TA-off operation. Upper and Lower denote the upper and lower experimental sampling locations and the corresponding numerical grid locations. Fast and slow data denote data taken at fast or slow kiln rotation rate, which has little influence on the measured baseline conditions. See also Figure 6.7.

<table>
<thead>
<tr>
<th></th>
<th>CO$_2$ (Dry Mole Fraction)</th>
<th>O$_2$ (Dry Mole Fraction)</th>
<th>Gas Temperature (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Upper</td>
<td>Lower</td>
<td>Upper</td>
</tr>
<tr>
<td>Model</td>
<td>0.069</td>
<td>0.005</td>
<td>0.084</td>
</tr>
<tr>
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Figure 6.7 Comparisons of model predictions with experimental data for TA-off operation. Upper and Lower location denote position at which the comparisons are made, as shown in Figure 6.6. Fast and Slow data are taken at different kiln rotation rates, however this does not influence conditions when no waste is being incinerated. Data are from Table 6.2.
rotary kiln incinerator (Cundy et al. 1989a, 1989b, 1989c, 1991a, 1991b; Chapters 3-5), and has been described as vertical stratification of species and temperature at the kiln exit. Even with the assumptions and approximations incorporated into the model, and the coarse nature of the grid, the model predictions show this vertical stratification quite clearly. The overall (gross) agreement between the model and the data is quite remarkable considering the limitations of the model and the uncertainties of the experimental measurements.

In spite of the good overall agreement with the experimental data, the shortcomings of the model are apparent. The model tends to overpredict the O$_2$ and underpredict the CO$_2$ at both locations. This may be caused by overestimation of the leak air flow rate, or the model may be under-predicting the mixing in the system. The model predicts much higher temperatures in the upper kiln and lower temperatures in the lower kiln relative to the experimental data. The very high temperatures are probably caused by neglecting radiation heat transfer in the model; the flame observed in the kiln during experiments was luminous and thus was losing substantial heat via radiation. An under-prediction of the mixing in the system may also explain why the model predicts more extreme temperatures than were experimentally measured. The coarseness of the numerical grid may contribute to the underprediction of mixing by making it impossible to resolve small eddies that may augment mixing in the real system. The model predicts a steep gradient in all variables at the upper sampling point, and the experimental location of the sampling probe tip is not known that accurately. Consequently, a small experimental error in probe tip location can cause a large discrepancy when comparisons are made, even if the model predictions are correct.
TA-on Results

A second baseline case model was solved for the conditions of turbulence air addition, since experimental data also exist for this operating condition. The vector components of the velocity are shown in Figure 6.8. Again, a high velocity jet originates near the burners and then turns up into the top of the kiln where it accelerates toward the exit. A large eddy is seen above the loading chute door, and reverse flow occurs in the bottom of the kiln in the center plane (X=8) near the kiln exit. The flow from the upper turbulence air nozzle is seen to turn downward even though the nozzle is angled upward. This is probably because the ambient turbulence air is much denser than the surrounding hot gas. The lower turbulence air nozzle flow appears to coalesce with leak air from the loading chute door as it flows along the floor of the kiln.

Figure 6.9 shows the temperature field at six slices across the kiln axis. The upper turbulence air nozzle is clearly visible in the first slice (Z=1), as are the loading chute door and the lower turbulence air nozzle. Progressing down the kiln (increasing Z), the jet from the upper turbulence air nozzle mixes with hotter gas as it drops toward the lower kiln. At all slices but the exit, the center of the flame zone appears cooler than its edges, which is to be expected because it is a diffusion flame. The kiln becomes highly stratified with high temperatures in the upper kiln, and this persists through to the kiln exit plane.
Figure 6.8 Vector velocity component plots for TA-on operation. These plots are vertical slices parallel to the center axis of the kiln (see Figure 6.3).
Figure 6.9 Gas temperature plots for TA-on operation. These plots are slices across the kiln axis at the specified axial locations (see Figure 6.3).
Model Verification—Comparison with Experimental Data

Experimental measurements were taken from the same locations shown in Figure 6.6 when turbulence air was added to the kiln. Table 6.3 shows the experimental measurements of O₂, CO₂, and gas temperature as well as the model predictions for these locations, while Figure 6.10 compares the model predictions with experimental data in a series of bar charts. Both the model and the data show high O₂, low CO₂, and low temperatures in the lower kiln, and low O₂, high CO₂, and high temperatures in the upper kiln. Similar to the comparisons made for operation without turbulence air, the model tends to overpredict the differences between the sampling points. In particular, for the upper sampling point the model predictions are rather far from the experimental data. The model does predict a very steep gradient in all variables at the upper sampling point, so experimental error in probe location may account for much of the discrepancy between the model and the experimental data. Overall, however, the model does predict the correct trend as a function of sampling location, and the agreement between the model and the experimental data is quite good considering the limitations of the model and the uncertainty of the field-scale measurements.

Table 6.3 Comparison of model predictions with measured data for TA-on operation. Upper and Lower denote the upper and lower experimental sampling locations and the corresponding numerical grid locations. Fast and slow data denote data taken at fast or slow kiln rotation rate, which has little influence on the measured baseline conditions. See also Figure 6.10.

<table>
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<th>O₂ (Dry Mole Fraction)</th>
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</tbody>
</table>
Figure 6.10 Comparisons of model predictions with experimental data for TA-on operation. Upper and Lower location denote position at which the comparisons are made, as shown in Figure 6.6. Fast and Slow data are taken at different kiln rotation rates, however this does not influence conditions when no waste is being incinerated. Data are from Table 6.3.
Comparison of TA-off vs. TA-on Model Results

One of the goals for this model is to learn how adding turbulence air influences the temperature, species, and flow-fields in the kiln. The model predictions for the flow-fields and temperature fields of the kiln for both operating conditions have already been presented. They show remarkable similarity regardless of the turbulence air addition. When turbulence air is added, the velocities are higher because the flow rates have been increased. The turbulence air model also shows a cool center in the flame zone that was not present without turbulence air. Figure 6.11 shows the O_2 mole fraction along the centerline of the kiln for operation both with and without turbulence air. The addition of turbulence air causes much lower O_2 levels in the flame zone of the upper kiln, and these lower O_2 levels are seen to persist through to the kiln exit plane. The gradient in O_2 near the kiln exit is also steeper when turbulence air is on, suggesting that the turbulence air, rather than promoting mixing, may be increasing stratification. A possible mechanism for this effect is seen in Figure 6.12, where the CH_4 mole fraction is shown along the centerline of the kiln for both operating conditions. The CH_4 is consumed near the burners during operation without turbulence air. In contrast, when turbulence air is added, substantial CH_4 remains in the upper kiln where the O_2 levels are near zero. The support burners produce a more fuel rich flame that becomes a purely diffusion flame in the upper kiln during turbulence air addition. The heat release from combustion near the roof of the kiln stabilizes the already stratified flow and minimizes subsequent mixing. In contrast, the support flame during TA-off operation releases most of its heat before it reaches the roof of the kiln, and the resulting hot gas moves upward due to buoyancy and promotes a limited amount of mixing.

This mechanism by which stratification increases during turbulence air addition suggests a reinterpretation of the experimental data presented in Chapters 3 and 4. In those chapters, the measured increase in O_2 at the upper kiln sampling point when turbulence air was turned on suggested that the turbulence air induced greater mixing.
Figure 6.11 Oxygen dry mole fraction plots for a) TA-off and b) TA-on operation. These plots are vertical slices along the center axis of the kiln (X=8).
Figure 6.12 Methane dry mole fraction plots for a) TA-off and b) TA-on operation. These plots are vertical slices along the center axis of the kiln (X=8).
between the O$_2$-rich gas in the bottom of the kiln and the O$_2$-depleted gas in the top of the kiln. However, turbulence air induced mixing should have also reduced the O$_2$ levels in the lower kiln, and this did not occur. Because the overall combustion stoichiometry for the kiln was the same in both cases, the measured increase in O$_2$ levels at the upper sampling point should have been accompanied by a decrease in O$_2$ levels elsewhere in the kiln exit flow, or an increase in unburned CH$_4$ elsewhere in the kiln exit flow, or both. Both model and visual observations suggest that low O$_2$ levels occur at the top of the kiln exit, above the upper sampling location. Thus, the experimental data are not inconsistent with the model's prediction that turbulence air addition can increase stratification if the support burners are operated in a more fuel-rich mode.

**PARAMETRIC STUDY**

In order to exercise the utility of the model and gain insight into the kiln operation, a numerical parametric study is undertaken. The baseline model with no turbulence air (TA-off) has been discussed, as was the baseline model with turbulence air on (TA-on). A list and discussion of the other parametric models based upon TA-off operation follows:

**TA-off**

- Baseline case
- No gravity
- All leak air enters through the loading chute
- No leak air enters through the ash sump

In the first parametric case (TA-off No gravity), the body force due to gravity is removed from the baseline TA-off model. Everything else remains exactly the same. This is intended to illustrate the importance of buoyancy on the model predictions.
The next parametric model (TA-off All leak air enters through loading chute) changes the location of the leak air entering the system. In this configuration, the total leak air flow rate from the TA-off baseline model is assumed to enter through the loading chute door, whereas only 35% was allowed in the baseline model. The leak rates through the front and rear seals, and the ash sump are all set to zero, while all other conditions are held the same. This parametric model may simulate conditions that occur in the actual rotary kiln when the loading chute door opens to admit solids.

The influence of the leak air assigned to the ash sump is determined in the next case (TA-off No leak air enters through ash sump). This case is identical to the baseline TA-off case except the ash sump leak rate is set to zero; to simplify the comparison, the other leak rates are not increased to replace this air. The primary interest in this case is whether flow recirculation through the kiln exit is being augmented by this input.

A set of parametric cases was also generated based upon the baseline TA-on model. These include:

**TA-on**
- Baseline case
- Turbulence air preheated to 433 K
- Turbulence air preheated to 900 K
- No leak air

First, a case was formulated where the turbulence air was preheated to 433 K (TA-on Turbulence air preheated to 433K). This temperature was selected based upon the temperature of steam available at the facility. In preheating the turbulence air, the turbulence air nozzle inlet velocities are increased to maintain the same mass flow rate of the lower density hot air. This case is intended to show whether preheating the
turbulence air can improve gas mixing by reducing its tendency to settle into the bottom of the kiln and by increasing its inlet velocity.

A second case is formulated to study preheating of the turbulence air (TA-on Turbulence air preheated to 900K), and is motivated by the inconclusive results of the previous case. In the second case, the turbulence air is preheated to 900 K, a temperature that may be possible using gas or electric air heaters. Again all other variables remained the same as the baseline TA-on case, but the turbulence air inlet velocities were increased to maintain the same mass flow rate of the hot, low density air.

The final parametric case (TA-on No leak) addresses conditions when no leak air is allowed to enter the system. This case would have been formulated with TA-off, as were the other leak studies, but the air present for combustion would have been much less than stoichiometric (63% theoretical air). The TA-on baseline case was used in this formulation because it contains enough metered air from the burners and TA nozzles to operate at 95% theoretical air, which is nearly stoichiometric. Thus, the leak air entering the system was completely turned off while all other variables remained the same as the baseline TA-on case.

To facilitate comparisons between the experimental cases, only the oxygen mole fraction and velocity are considered. For the cases based upon TA-off, Figure 6.13 presents vertical slices along the center axis of the kiln showing oxygen mole fraction, while Figure 6.14 shows oxygen mole fraction in horizontal slices along the kiln axis for selected TA-off cases. Figure 6.15 shows the axial velocity at the kiln exit plane for the TA-off cases. For the cases based upon TA-on, Figure 6.16 presents vertical slices along the center axis of the kiln showing oxygen mole fraction, Figure 6.17 shows oxygen mole fraction in horizontal slices along the kiln axis for selected TA-off cases, and Figure 6.18 shows the axial velocity at the kiln exit plane. These six figures will be referred to repeatedly in the following discussions.
Figure 6.13 Oxygen dry mole fraction plots for TA-off operation. These plots are vertical slices along the center axis of the kiln (X=8).
Figure 6.14 Oxygen dry mole fraction plots for TA-off operation. These plots are horizontal slices along the center axis of the kiln (Y=8). The dashed line shows the kiln exit plane; the transition section begins below the line.
Figure 6.15 Axial (Z component) velocity plots for TA-off operation. These plots are vertical slices across the center axis of the kiln at the kiln exit plane (Z=28). Positive velocities are represented by the gray scale, while zero and negative velocities are represented by the solid contour lines. The first solid contour line represents zero axial velocity, and each subsequent line represents an increment of 0.5 m/s in the negative Z direction (flow toward the burner face).
Figure 6.16 Oxygen dry mole fraction plots for TA-on operation. These plots are vertical slices along the center axis of the kiln ($X=8$).
Figure 6.17 Oxygen dry mole fraction plots for TA-on operation. These plots are horizontal slices along the center axis of the kiln (Y=8). The dashed line shows the kiln exit plane; the transition section begins below the line.
Figure 6.18 Axial (Z component) velocity plots for TA-on operation. These plots are vertical slices across the center axis of the kiln at the kiln exit plane (Z=28). Positive velocities are represented by the gray scale, while zero and negative velocities are represented by the solid contour lines. The first solid contour line represents zero axial velocity, and each subsequent line represents an increment of 0.5 m/s in the negative Z direction (flow toward the burner face).
**TA-off Parametric Cases**

**TA-off Baseline Case**

For comparison purposes, the baseline TA-off case is shown in Figure 6.13-a. The flame (low oxygen region) is seen to rise from its origin on the right, then flow along the top of the kiln toward the exit. A clockwise eddy is seen in the upper right of the figure, where low oxygen gas is drawn back toward the base of the burner flames. Notice that even near the top of the kiln, the oxygen levels never drop below approximately 2%. This is because mixing and diffusion have been sufficiently rapid to satisfy combustion oxygen requirements. Figure 6.14-a shows a horizontal slice along the kiln axis for the baseline TA-off case. The burner inlet is on the upper right. Low oxygen regions appear on the edges of the burner jet where mixing with leak air augments the combustion. The flame then rapidly rises through this plane toward the top of the kiln, and only high oxygen levels are seen for the rest of the kiln. The small jet of low oxygen on the upper left is due to the sludge lance inlet, where a small amount of steam (with zero oxygen content) is admitted to keep the nozzle cool. Figure 6.15-a shows the flow stratification and the large area of reverse flow through the kiln exit plane (Z=28).

**TA-off No Gravity**

In Figure 6.13-b, the case with no gravity is presented. It shows very graphically a lack of vertical stratification compared to the baseline case. The jets from the two support burners originate on the right, broadening and coalescing as they approach the center of the kiln. Keep in mind that substantial leak air enters the lower kiln through the loading chute door and the ash sump, causing generally higher oxygen levels in the lower kiln. The flame does tend to curve upward as it reaches the kiln exit plane before turning and exiting the computational domain vertically. Clearly, in
comparison with Figure 6.13-a, buoyancy of hot gases is extremely important in producing the stratified flow observed in the baseline case and in the experimental data. Further insight may be gained from Figure 6.14-b, where a horizontal section shows the flame originating at the burners on the upper right. The flame expands as it flows along the kiln, but it tends to remain on the burner side of the kiln. This is very different from the baseline case (Figure 6.14-a), where the flame rapidly passes through the center plane as it rises into the upper kiln, and the rest of the center plane has very high oxygen levels. Figure 6.15-b shows that the flow through the kiln exit plane is much less stratified than the baseline case, and the zone of recirculation is greatly reduced.

TA-off All Leak Air Enters Through Loading Chute Door

Figure 6.13-c shows the case in which all the leak air enters through the loading chute door. The cold, dense leak air immediately drops into the bottom of the kiln and persists with little mixing until it reaches the transition section. Consequently, along the top of the kiln, the flame oxygen requirements are not satisfied as readily and a large oxygen deficient region is formed. The recirculation zone in the upper right of Figure 6.13-c is still visible, but note that it brings gas containing no oxygen to the front wall of the kiln to be entrained in the upper burner jet. In the baseline case, air entering the front seal mixes in this eddy and delivers more oxygen to the upper burner jet. Figure 6.14-c appears similar to Figure 6.14-a, showing that the change in leak air location had little effect on the lower burner as the lower half of the kiln is rich in oxygen in both cases. Figure 6.15-c shows that the leak air entering through the loading chute door displaced the recirculation zone at the kiln exit plane. In the baseline case, substantial reverse flow existed at the bottom of the kiln exit, while in this case the bottom of the kiln exit is occupied by air flowing directly from the loading chute door along the floor. As a result, only two small regions of recirculation are observed at the
sides of the kiln exit, each well above the kiln floor and the larger of the two on the side opposite the burners.

**TA-off No Ash Sump Leak Air**

Figure 6.13-d is nearly identical to Figure 6.13-a except that the high oxygen layer in the bottom of the kiln is thinner. In the baseline case, air leaking into the sump enters the kiln and flows upstream along the floor of the kiln, and this is not possible when no sump leak is present. From Figure 6.15-d, one sees that recirculation across the kiln exit plane was reduced without the sump leak air flow, but it was not completely eliminated as might be expected.

**TA-on Parametric Cases**

**TA-on Baseline Case**

Figure 6.16-a shows the baseline TA-on case for comparison purposes. Compared to the baseline TA-off case (Figure 6.13-a), oxygen levels are much lower in the top of the kiln, and the vertical gradient in concentration is greater. The cause of these conditions, support burners operating in a more fuel rich condition relative to the TA-off case, was discussed previously. The eddy in the upper right corner is visible, and leak air from the seal is seen to augment the oxygen levels there. The figure does not show any evidence that the turbulence air enhances gas-phase mixing. A horizontal section through the kiln in Figure 6.17-a is quite similar to the baseline TA-off case in Figure 6.14-a. The support flame, however, is noticeably longer and its oxygen levels are lower before it passes through the center plane and rises into the upper kiln. Part of this effect may be due to the higher velocities from the support burners because the burner flow rates are higher when the turbulence air is on. Also, the lower turbulence air nozzle, being below the lower burner, may draw the flame down
somewhat before buoyancy forces it up through the center plane. **Figure 6.18-a** shows a similar flow pattern to that obtained with the baseline TA-off case (**Figure 6.15-a**). The recirculation zone in the bottom of the kiln is very comparable in size and magnitude, but the TA-on case shows higher velocities near the top of the kiln.

**TA-on 433 K Preheat of the Turbulence Air**

**Figure 6.16-b** shows the case with the turbulence air preheated to 433 K. Very little effect is seen relative to the baseline TA-on case in **Figure 6.16-a**. Preheating the turbulence air should augment mixing because it would have higher jet velocities and it would be less dense, therefore it would have less tendency to sink to the floor of the kiln. However, relative to the flame temperatures, preheating the turbulence air from 300 K to 433 K appears to make little difference. Also, relative to the amount of leak air entering the system, the turbulence air flow is small so it cannot reduce the overall buoyant stratification. This is seen clearly in **Figure 6.18-b**, where the flow pattern is almost identical to that of the baseline case in **Figure 6.18-a**.

**TA-on 900 K Preheat of the Turbulence Air**

A more drastic preheat of the turbulence air, to 900 K, is shown in **Figure 6.16-c**. Here, the low oxygen region along the top of the kiln has been reduced substantially in extent. The dark horizontal streak where the flame normally appears is a region of higher oxygen levels originating from the upper turbulence air nozzle. In the lower right of the kiln, the region of slightly reduced oxygen levels is seen to dip closer to the kiln floor. This is the effect of the lower turbulence air nozzle entraining products from the support flame and mixing them with the air in the lower kiln. The oxygen concentration gradient is less severe than in **Figure 6.16-a**, and this condition persists through the kiln exit plane. However, the degree of stratification at the kiln exit is still no better than observed in the baseline TA-off case (**Figure 6.13-a**). **Figure 6.17-b**
shows the horizontal section through the center of the kiln for this case. The lower burner flame persists below the centerline substantially longer than in the baseline TA-on case (Figure 6.17-a). This is evidence that the lower turbulence air nozzle is drawing the flame down into the lower kiln, and the higher velocities of the preheated turbulence air augment this process. Also, a more extensive region of lower oxygen levels is visible in the front half of the kiln, as the lower turbulence air nozzle mixes some combustion products into this region. The flow pattern at the kiln exit plane, shown in Figure 6.18-c, again shows clearly that stratification has not been substantially reduced. The flow pattern shows a broader region of outward flow than the baseline case, but it also has a slightly more intense recirculation zone at the kiln exit.

**TA-on No Leak Air**

Figure 6.16-d shows the case where no leak air enters the kiln; the only air enters through the burners and the turbulence air nozzles. The overall stoichiometry for the kiln in this case is 96% theoretical air, so oxygen levels are generally low. Still, the lower turbulence air jet persists along the floor of the kiln. The vertical section does not show the true nature of the solution; Figure 6.17-c gives the horizontal section through the center of the kiln. Here, oxygen is consumed on the burner side (right) of the kiln, while oxygen from the turbulence air nozzles persists on the other side (left) through the kiln exit. When leak air is not present in the system, stratification in the vertical direction due to buoyancy is greatly reduced. This is replaced by segregation in the horizontal direction originating with the different entry locations of the air and natural gas. Where natural gas and air come into contact, high temperatures result and buoyancy causes an upward flow. However, the amount of combustion actually occurring is small, and the resulting hot gas quickly mixes with the surrounding gas, limiting the stratification. This situation persists through the kiln exit, shown in Figure 6.18-d, where the contact layer between natural gas and air corresponds with the
highest flow velocities on the left. The reverse flow on the right persists nearly to the front of the kiln, but it is devoid of oxygen and does not augment combustion of the natural gas from the support burners.

SUMMARY AND CONCLUSIONS

A detailed numerical model of an industrial rotary kiln incinerator is formulated and solved using a commercial finite difference code. Two baseline cases are tested (turbulence air on and off) and the results are analyzed for qualitative features in locations where experimental measurements have been unobtainable. The model predictions are shown to be physically realistic by comparison with experimental measurements obtained in the industrial rotary kiln that was modeled. Comparisons are made at only specific locations where experimental measurements have been taken. The overall conclusions concerning the quality and utility of the model predictions are:

• Both baseline model cases predict qualitatively the gradient in temperature and species concentrations that have been measured experimentally near the kiln exit.

• Quantitative agreement between the predictions of both baseline model cases and experimental data is relatively good at the lower experimental location but poor at the upper experimental location. The models' predictions of very steep gradients near the upper sampling location, combined with experimental uncertainty in the location, may account for this poor agreement.

• A comparison between the baseline model cases suggests that the addition of turbulence air may increase stratification in the kiln rather than augment bulk gas phase mixing. The mechanism for this behavior appears to be the increased natural gas flow rates used when operating with turbulence air on, causing a
more fuel rich support flame. This fuel rich, diffusion limited, support flame consumes fuel more slowly and releases more of its heat near the top of the kiln, augmenting the thermal stratification.

- A reinterpretation of the experimental data in Chapters 3 and 4 suggests that the turbulence air addition may be increasing stratification as the model predicts, rather than improving mixing as has been suggested based upon experimental data alone. Although this cannot be shown conclusively with existing data, it deserves further investigation.

In analyzing the qualitative features predicted by the baseline model cases, the following observations are made:

- The flow field predicted by the model for both baseline cases shows the hot support flame rising rapidly to the top of the kiln and proceeding along the ceiling toward the exit.

- In both baseline model cases, the leak air is seen to drop to the bottom of the kiln and flow along the kiln floor.

- In both baseline model cases, some flow proceeds upstream through the kiln exit and along the kiln floor before it meets an opposing flow of cool air from the front of the kiln.

- In the model case with turbulence air on, the jets of cool turbulence air rapidly turn downward and drop toward the bottom of the kiln.
Once the baseline model cases are analyzed and their utility demonstrated, a numerical parametric study is performed. The parametric study addresses the importance of buoyancy on the flow field, the influence of leak air location and quantity, and the effects of preheating the turbulence air. The following conclusions are drawn:

- Buoyancy of the hot gases is indeed the primary cause of the observed vertical stratification in the kiln.

- Decreasing the leak rate through the front seals appears to starve the support flames for oxygen. This is because much of the support flames' oxygen is entrained at the base of the burners on the front wall of the kiln, where air leaking through the front seals is available.

- Increasing the leak rate through the loading chute door causes more cool air to flow along the kiln floor at higher velocities, and it displaces the recirculation zone at the kiln exit from the bottom to the sides of the kiln.

- Eliminating leak air entering through the ash sump reduces the amount of recirculation at the kiln exit and displaces the recirculation zone upward.

- Completely eliminating all leak air while maintaining turbulence air addition drastically reduces buoyancy driven stratification, and the flow field becomes horizontally segregated into support flames on the burner side of the kiln and turbulence air on the other side.
Preheating the turbulence air to 433K has little effect. Preheating the turbulence air to 900K improves the gas phase mixing somewhat; however, the stratification at the kiln exit is similar in degree to that observed with TA-off.

Overall, this modeling study has met its goals of improving our understanding of the flow field within the kiln and the influence of selected parameters on this flow field. The model has been successful in predicting qualitative trends observed experimentally, and it has provided a valuable tool to help interpret the limited experimental data available. This work has demonstrated that a detailed numerical model of intermediate complexity can be sophisticated enough to provide very useful, although not quantitatively exact, results while remaining manageable enough to be readily handled by available numerical codes and inexpensive computers.

Future rotary kiln modeling efforts will proceed along two avenues. One avenue will explore the use of similar, intermediate complexity models to address more difficult problems such as the time dependent flow field resulting from transient waste incineration. Another avenue will be to keep the focus on steady-state kiln operation with methane support flames only, while improving grid resolution and addressing radiation heat transfer. We hope that these future efforts, together with improved numerical methods and better computer hardware, will soon lead to a more reliable and comprehensive predictive capability for rotary kiln incinerator performance.
CHAPTER 7

BED MIXING AND HEAT TRANSFER IN A
BATCH-LOADED ROTARY KILN

INTRODUCTION

Rotary kiln incineration is one method often used to destroy hazardous waste. This is a complex process involving many simultaneous heat and mass transfer phenomena. For waste adsorbed on solid materials, the desorption rate of the waste is of particular importance. The ability to predict the transient desorption or evolution rate of waste is necessary for proper design and operation of a kiln and afterburner system. The system must be designed and operated such that the instantaneous evolution rate never exceeds the capacity to destroy effectively the evolved waste, thus avoiding an event referred to as a transient "puff" (Linak et al. 1987a, 1987b; Wendt and Linak 1988). Also, prediction of the transient evolution rate, when combined with the residence time distribution of the solids in the kiln, allows the estimation of the residual contamination on the ash exiting the kiln.

Rotary kilns are capable of processing many types of waste (solids, liquids, or mixtures of solids and liquids) under a variety of loading conditions. This research is concerned specifically with the processes involved in the incineration of periodically loaded liquid wastes adsorbed on solids. The difficulties in predicting evolution rates can be better understood by reviewing the sequence of events that occurs during this incineration process. On the basis of video images as well as temperature and species concentration measurements near the exit of an industrial-scale rotary kiln incinerator.
Cundy et al. (1991b) and Cook et al. (1992) describe the incineration of periodically fed waste in a rotary kiln. The surrogate waste used in these experiments is either xylene or dichloromethane adsorbed on clay. These wastes are initially contained in plastic containers, or packs. As a new pack is introduced into the kiln (once every ten minutes), it falls on a hot bed of relatively clean solids remaining from previous packs. The new pack is heated by energy transferred from the support flame, the hot combustion gases, the kiln walls, and the bed of solids. Within about 30 seconds the plastic pack disintegrates and the sorbent begins to mix with the existing bed in the kiln. As the sorbent begins to heat, the volatile waste species desorbs and is incinerated.

In this paper, we review previous bed evolution studies, as well as other work dealing with the description of and prediction of bed motion and heat transfer to rotary kiln beds. Experiments that demonstrate the importance of mixing on the heat transfer to periodically fed solids are discussed. Results of these experiments lead to a relatively simple model that predicts the heating of the solids including the effects of mixing.

**Evolution of Waste from Solids**

Several attempts have been made to measure and to model desorption rates in pilot-scale rotary kiln simulators. In one such study, Linak et al. (1987a) measured evolution characteristics and puff generation with batch fed solid wastes in a pilot-scale rotary kiln simulator. The simulator is a 73 KW directly fired unit with dimensions of 0.762 m inside diameter and 0.61 m length. The authors used statistical response surface techniques to select test conditions for parametric studies. They selected charge mass, charge surface area, kiln temperature, and waste material as the independent variables. The waste charges consisted of a number of plastic rods of varying lengths to give the desired mass and surface area. The rods consisted of high density polyethylene, low density polyethylene, polyvinyl chloride, and polystyrene plastics. The dependent variables were transient peak height of the total hydrocarbon analyzer sampling the kiln
exhaust gas, and the total area under each transient peak. The results of the experiments were statistically analyzed to produce response surfaces of the dependent variables. The authors concluded that increasing the kiln temperature may increase the peak height but decrease the area under the peak, thus decreasing the integrated mass of hydrocarbons exiting the kiln. Both peak height and integrated mass were strong functions of the mass and surface area of the charge. The authors suggest that the formation of transient puffs results from a complicated mixture of physical and chemical processes in the kiln. The processes appear to be strongly dependent on the nature of the solid waste, the heat transfer to the solid waste, the rate of waste vaporization, and the gas phase stoichiometry.

Linak et al. (1987b) also discuss the incineration of liquids bound on solid sorbent material contained in cardboard containers, using the same pilot-scale rotary kiln described previously by Linak et al. (1987a). In these tests, the waste charges consist of toluene, dichloromethane, carbon tetrachloride, or No. 5 fuel oil adsorbed onto ground corncob material contained in 0.95 L cylindrical cardboard cartons. Parametric studies were performed using statistical response surface methods. The independent variables were kiln temperature, liquid charge mass, and kiln rotation rate, while the dependent variables were total hydrocarbon peak height and area. Increases in any of the three independent variables led to increases in both of the dependent variables. Difficulties in data interpretation owing to the nonlinear response of the total hydrocarbon analyzer are discussed, as well as the problem of determining the appropriate puff indicator (THC, CO, soot mass) for each waste species. The speciation of the exhaust gas is reported for each of the waste species tested. The authors suggest that the volatile release rate is probably controlled by heat transfer, surface exposure, contaminant vapor pressure, and heat of vaporization of the contaminant.

Wendt and Linak (1988) proposed a theoretical model to predict waste evolution and puff formation from batch loaded liquid wastes bound on ground corncob sorbent
material. The proposed model relates desorption rate to vapor pressure through the Clapeyron equation, and to surface area. They assume that the surface area follows a fragmentation type behavior in which the solids periodically fragment to produce two pieces out of every one. The rate of fragmentation is assumed directly proportional to the kiln rotation rate. The model appears to simulate the salient features of the experimental runs, including multiple evolution peaks, but it fails to agree quantitatively without adjustment of the parameters.

Owens et al. (1992) performed studies on toluene adsorbed on montmorillonite clay particles. Charges of this waste were fed into an empty pilot-scale rotary kiln simulator where the toluene vaporized without combustion and was measured in the kiln exhaust gas. The independent variables for the study were kiln wall temperature, solids fill fraction, and kiln rotation rate. The bulk temperature of the solids was measured continuously with a thermocouple immersed in the bed of solids. The time-varying desorption rate of toluene was calculated from the exhaust gas flow rate and the measured toluene concentration in the exhaust gas. These data were interpreted in terms of a surface renewal model. The model assumes that the bed is periodically well mixed, with depletion of toluene occurring on the exposed surface during the stationary intervals. This draws conceptually upon the observed slumping motion of the bed, where the surface of the solids is stationary until a slump occurs and the surface is renewed. The slumping frequency was determined experimentally as a function of fill fraction and rotation rate, and was then incorporated into the model. The rate of toluene desorption was determined by the rate of diffusion through the surface layer, which is approximated as a semi-infinite medium; an effective diffusion coefficient with an Arrhenius-type dependence on temperature was used. The resulting model has two empirical constants that were adjusted to give the best fit of the data. The temperature in the Arrhenius term is supplied by the measured bed temperature (assuming the bed to be spatially isothermal) as a function of time. Because the model is exponentially dependent upon temperature, the
predicted evolution rates are highly sensitive to the temperature of the solids. The predicted toluene evolution rates agree surprisingly well with those determined experimentally, although the two fit parameters were temperature dependent.

**Bed Mixing and Heat Transfer Considerations**

Bed evolution studies suggest that evolution rates are dependent on many parameters including waste and sorbent properties, bed motion, and heat transfer considerations. The process of contaminant evolution from the solid material is greatly accelerated by heat transfer to the bed material. It should be noted that current rotary kiln incinerator models assume that the bed is thermally and materially well mixed in the radial and circumferential directions (Owens et al. 1991). Variation is allowed only in the axial direction, resulting in a one-dimensional bed model. These models are generally based upon an assumption of steady-state solids feed, so the transient nature of the problem is eliminated. While some of these models have been successful in describing steady-state phenomena in rotary kilns, they are not capable of predicting evolution from periodically loaded waste. That is, even if the assumption that the bed is essentially well mixed is justified, these models will fail when that assumption is applied to freshly fed solids.

To describe fully the heat transfer to the cold waste material introduced onto hot bed material, bed motion and mixing as well as external heat transfer to the bed must be considered. These considerations provide a foundation for understanding bed mixing and how it influences bed heat transfer and waste desorption rates.

The characteristics of particle motion in rotating drums have been previously investigated (Lehmberg et al. 1977; Henein et al. 1983a, 1983b). Lehmberg et al. (1977) placed dyed particles on an existing bed of a rotary drum and observed the resulting particle motion through the transparent end of the drum. Based on these experiments, the authors describe the bed as consisting of two distinct regions. The first region contains particles that are stationary relative to the rotating drum wall. The particles in this region
follow the wall up to some critical height then they roll down the exposed surface of the bed. The moving particles at or near the surface of the bed constitute the second region that the authors term the well-mixed layer of the bed. The authors qualitatively describe the mixing process by which the dyed particles are distributed throughout the bed. To quantify the mixing rate in the rotating drum, the authors measured the transient temperature at a point in the bed after a charge of relatively hot material was added to the drum. A characteristic decay time constant was determined for the process of equilibrating the bed temperature. These experiments demonstrated that the decay time of the system decreased as the drum rotation rate increased.

Henein et al. (1983a) has more completely described the possible bed motion in a rotary kiln. The authors describe the four regimes of bed motion typically found in rotary kilns: slipping, slumping, rolling, and cascading. Cascading motion is characterized by relatively high rotation rates where particles are thrown free of the wall and follow a ballistic trajectory before reentering the stationary layer against the wall. At lower rotation rates, rolling motion occurs in which particles continuously pass through the mixing layer and the free surface is flat and moves constantly. At still lower rotation rates, the motion is similar except that the free surface only moves intermittently. This is termed slumping motion. Under special conditions where the bed tends to stick together, the entire bed intermittently slips relative to the wall. In this motion regime, called slipping, little or no mixing occurs and the free surface contains the same material for long periods of time. Through a series of experimental investigations the authors find the operating conditions and bed properties that result in the various types of bed motion. In general, the bed motion is found to be influenced by the fill fraction, kiln rotation rate, kiln diameter, and sorbent particle diameter. A semi-empirical model is developed to predict the bed motion based on these parameters. With the possible exception of some slipping bed motions, the bed motion modes typically encountered in rotary kilns follow the conceptual model of
Lehmberg et al. (1977) in which a layer of solids near the wall is stationary relative to the wall and an outer layer where mixing occurs.

With information about the motion of the bed material, one can gain some insight into how heat is transferred to the bed. In general, many factors may influence the transfer of heat to the bed in a rotary kiln (Barr et al. 1989a, 1989b). However, under the special operating conditions of low temperature, no radiant flame, and low gas phase flow rates, heat conduction from the portion of the kiln wall in contact with the bed becomes the dominant mode of heat transfer to the bed (Owens et al. 1991). The conduction occurs through the stagnant layer of the bed as it moves with the kiln wall. Several investigators, including Tscheng and Watkinson (1979), have developed empirical heat transfer coefficients for this conduction process. These coefficients generally depend on kiln rotation rate, bed material properties, and a film resistance between the wall and the bed material. Thus the heat transfer to the bed from the covered wall can be described by a single heat transfer coefficient and the temperature difference between some characteristic temperature of the bed material and the wall temperature. This characteristic temperature is usually taken to be that of the assumed well-mixed bed. However, if the bed is not well mixed it is not clear what bed temperature should be used with such a heat transfer coefficient in calculating heat transfer from the wall. That is, the heat transfer from the kiln wall is itself dependent on the mixing of the bed.

The rate at which the cold solids are heated by mixing with the hot solids is critical in determining the initial rate of waste evolution in many practical incinerator applications. Clearly if the initial mixing process takes minutes, the well-mixed bed assumptions may fail to predict accurately the heat transfer from the kiln to the bed. However, in this case, the heat transfer to the cold sorbent due to mixing may be relatively slow and perhaps negligible. What is less clear is the opposite extreme, where the bed is justifiably assumed to be well mixed. If fresh sorbent is mixed with the hot sorbent in only a few seconds, then the initial rate of heat transfer due to mixing must be very high. Since heat
transfer drives the rate of evolution, this rapid mixing period may be accompanied by extremely rapid evolution, possibly resulting in an overload condition in the afterburner.

Clearly the mixing process influences heat transfer to the bed and heat transfer within the bed, and thus may significantly affect waste evolution rates. However this mixing process is poorly understood. The experiments described in the following discussions were designed to provide a better understanding of the bed mixing that occurs in a batch-fed kiln.

EXPERIMENTAL FACILITY

A series of experiments was performed using the pilot-scale rotary kiln simulator at the University of Utah. This facility has been described in detail by Lemieux and Pershing (1989), and is shown in Figure 7.1. It consists of a horizontal, refractory lined, rotating drum with internal dimensions of 61 cm long by 61 cm diameter. A natural gas/air support burner supplies heat to the system. One end of the drum is seated against a stationary exhaust section, which contains the kiln exhaust duct, a loading gate, a viewport, and fittings for the introduction of various probes into the system. To facilitate loading, a trough shaped loading chute is inserted through the loading gate. Waste is fed through the gate and down the chute. The waste lands inside the kiln near its center, the chute is retracted, and the gate is closed. The simulator differs from an actual rotary kiln incinerator in that the solids do not travel through the simulator, and they do not exit the system unless they are removed.

Since the present study does not presume the bed to be well mixed, a thermocouple probe was designed to measure simultaneously the bed temperature in several locations. The probe contains 4 thermocouples spaced 5 cm apart along the axis of the kiln. A diagram of this thermocouple rake is shown in Figure 7.2. The rake uses type K thermocouples in 0.3175 cm stainless steel sheaths. The sheaths are 91 cm long to reach from the port in the exhaust section into the bed. The thermocouples are
Figure 7.1 Plan view and cross section of the pilot-scale rotary kiln simulator at the University of Utah from Owens et al. (1992).
further supported by 0.635 cm stainless steel tubes that enclose them to within 1.27 cm of each thermocouple tip. The extra support is necessary to keep the thermocouple tips accurately positioned within the bed of solids, which tends to drag on the thermocouples. All of these tubes are bundled together inside a short piece of 1.9 cm stainless tube and the spaces between the tubes are sealed with refractory cement. This large portion of tube passes through the bulkhead and is held in place using standard tubing connectors. The thermocouple tips are positioned so that they are uniformly 1.27 cm away from the kiln surface and are approximately along the centerline (line of greatest thickness) of the bed. An additional thermocouple probe of similar design but containing a single thermocouple was left in place from earlier studies (Owens et al. 1991), thus providing a total of 5 thermocouples in the bed. The tip of the single thermocouple was located between the second and third thermocouples of the rake as shown in Figure 7.2.

Figure 7.2 Thermocouple rake for bed temperature measurements in the kiln simulator.
EXPERIMENTAL PROCEDURE

A set of experiments to simulate the mixing and heat transfer in a rotary kiln sorbent bed was developed as follows. First, it was decided that no desorbing waste should be included in these tests because it adds complexity. The desorption of waste takes heat from the bed, and so the heat and mass transfer are coupled. For these tests, the limit where heat and mass transfer are uncoupled is investigated, as there is no mass transfer in these experiments. The resulting heat transfer is a realistic approximation for sorbents containing low concentrations of waste species.

The main thrust of these tests is to study the thermal behavior of cold sorbent added to a hot sorbent bed. In field-scale rotary kiln incinerators, the waste is often loaded in containers that break down upon heating. This pack breakdown is another complicated process, which will eventually have to be addressed to make any evolution model physically realistic. Since the main purpose of this work is to study the mixing characteristics of the bed, this additional complication was removed by loading the sorbent into the rotary kiln simulator with no container. This eliminates the random effects of pack breakdown and yields more reproducible results.

In previous work, Owens et al. (1991) has shown that the predominant mode of heat transfer to the sorbent bed at relatively low temperatures is through contact with the hot kiln wall; the other modes of heat transfer, such as surface convection with the hot gas or radiation from the support flame and walls, are secondary. For this study, a baseline kiln temperature of approximately 360°C was chosen. This temperature was achieved using a non-luminous support flame with low gas flow rates. Under these conditions, convection heat transfer with the gas and radiation heat transfer were negligible. This simplifies the experiment to one of single-mode heat transfer between the kiln wall and solids.

Since the solids do not flow through the rotary kiln simulator, one can control fill fraction simply by measuring the volume of solids fed into the system, independent of
rotation rate. The sorbent material used in this study is commercially available calcined montmorillonite clay, consisting of irregular granules approximately 2 mm in diameter. For this study, measurements were performed at 1.5%, 3%, 4.5%, and 6% fill fractions. Larger fill fractions were not studied due to their exceedingly long heat up times. The kiln rotation rates were independently varied at 1.6, 0.8, 0.4, and 0.2 rpm. The observed bed motion was in the slumping regime for all conditions tested, except those at 1.6 rpm where rolling motion was exhibited. Because slumping and rolling motion are very similar except for the intermittent nature of slumping, this transition should have no effect on the mixing and heat transfer.

The experiments were performed using the following procedure. Charges of clean, dry, room temperature sorbent each weighing 1550 grams (each representing a fill fraction of 1.5% of the kiln) were prepared. The kiln was empty, at a steady-state wall temperature of 360°C, and the rotation was set at 1.6 rpm (near its fastest setting). One charge of sorbent was fed into the system, yielding a fill fraction of 1.5%, and its temperature response was monitored until it was near the steady-state temperature. Another charge was then introduced into the system on top of the hot sorbent, yielding a total fill fraction of 3%. The bed temperatures were again monitored until steady-state conditions were approached. This was repeated for a third charge (yielding 4.5% fill fraction), and a fourth charge (yielding 6% fill fraction). After the fourth charge reached steady state, the bed was vacuumed out and the rotation rate was decreased to 0.8 rpm. Four more charges were introduced in the same manner at the new rotation rate. This procedure was then repeated at rotation rates of 0.4 and 0.2 rpm. To approach steady state within a few degrees generally required between 10 and 30 minutes for each charge. During these measurement periods, the 5 thermocouple readings were recorded once every 2.5 seconds using a Macintosh SE computer with an Omega data acquisition package. In all, 16 sets of data were recorded.
Data Analysis

The resulting temperature traces showed some expected features, including the observation that it takes longer to heat up the bed if the fill fraction is increased or if the rotation rate is decreased. However, there were some surprising features as well. Oscillations in the temperature readings were observed for all conditions except the 1.5% fill fraction data, where sorbent was charged into an empty kiln. These oscillations were presumably from the cold sorbent and hot sorbent alternating contact with the thermocouples. As the hot and cold sorbent tumble within the kiln, they mix together and the oscillation decays until the sorbent reaches a uniform temperature. A typical temperature trace is shown in Figure 7.3 for a single thermocouple. It was noted further that these oscillations appear to decay more slowly at lower rotation rates, and that their period appears to increase as the rotation rate decreases. Other observations were that the thermocouple on the end of the rake farthest from the center of the bed often registered little or no response from the feeding of each charge, while the thermocouple nearest the center of the bed usually showed the greatest response. This was not totally unexpected because each new charge of loose sorbent tends to land near the center of the bed. Note, however, that the loading is done by hand and is subject to unavoidable variation.
Figure 7.3 Typical bed temperature trace showing oscillatory response and transient heating for kiln rotation rate of 0.8 rpm and 3% fill fraction.

An examination of the typical temperature trace shows that it is composed primarily of two parts. Overall, the temperature follows an exponential heat-up curve that can be characterized by some bulk heating time constant. This time constant describes the heat up of the bed if the bed is assumed to be well mixed. Superimposed upon the heat up curve is the sinusoidal oscillation with its associated period and decay constant. Although the decay of the oscillations may be due to both mixing of the bed particles and conduction through the bed, calculations given in Appendix B show that this decay constant is primarily a measure of the mixing in the bed. The period of the oscillation appears to be representative of the time necessary for a particle in the bed to rotate through the bed and return to the same position. This can also be described as the rotational period for the bed. This is not to be confused with the slumping period associated with
the periodic slumps in which solids traverse the free surface of the bed, nor with the rotational period of the entire kiln.

By combining these observed features we obtain an equation that is capable of describing the data curves in terms of these physically meaningful variables. The function is suitable for numerical curve fitting of the data to extract systematically the useful information, in particular the two time constants and the bed rotational period. The general form of the function is:

\[ T = A + B \cdot \exp\left( -t / \tau \right) + D \cdot (C + \sin(2\pi t / P + \phi)) \cdot \exp\left( -t / \theta \right) \]  

Where:
- \( T \) = temperature measured experimentally in the bed (K)
- \( t \) = time (seconds)
- \( \pi = 3.1415926 \)

The fitted parameters are:

- \( A \) = the final asymptotic temperature (K)
- \( B \) = the maximum change in \( T \) for the exponential heat up curve (K)
- \( C \) = the offset of the sinusoidal component superimposed on the curve
- \( D \) = the maximum amplitude of the sinusoidal component (K)
- \( \tau \) = the bulk heating time constant (seconds)
- \( P \) = the period of the sinusoidal oscillation (seconds)
- \( \phi \) = the phase shift in the oscillation (±π radians)
- \( \theta \) = the time constant for the decay of the oscillation (seconds)

Parameters such as the offset, \( C \), and the phase shift, \( \phi \), were introduced to allow the general function to fit each temperature curve. The resulting equation has one complicating quality: \( T \) is not a linear function of the parameters \( \tau, P, \phi, \) and \( \theta \). Therefore, methods for ordinary least-squares curve fitting cannot be applied. Rather, a
The parameters obtained by fitting the experimental data show interesting trends as functions of fill fraction and kiln rotation rate. Presentation of these data is difficult owing to the number of data points and the three independent variables: rotation rate, fill fraction, and axial location of each thermocouple. Figure 7.4 shows the bulk time constant as a function of these three independent variables. The vertical axis is the bulk time constant in seconds. The horizontal axis is not discrete, and is divided into four regions containing data obtained at each kiln rotation rate. Each of these regions is further divided into four regions containing data obtained at each fill fraction. Within each of these fill fraction divisions are the four data points representing the four thermocouples in order of decreasing distance from the kiln centerline. Although five thermocouples were used in the experiments, the one farthest from the centerline showed very little temperature response and the general function did a poor job of fitting this data. For these reasons, only the fitted parameters obtained from the other four thermocouples are included in further analysis. Some other curve fits were rejected because the fits were poor. In particular, at slow rotation rates the fitted values of the bulk time constants (τ)
were very large and were associated with fitted values of the final asymptotic temperature (A) much greater than the actual kiln wall temperature of 360°C, which is physically unrealistic. This occurred because only the first 600 seconds of the data were used in obtaining the curve fits, and for slow rotation rates and large fill fractions the transient temperature was not yet near its asymptotic value after only 600 seconds. Data obtained at 1.5% fill fraction are obviously missing all the parameters associated with the sinusoidal component. This component was not present in the data because there was no preexisting bed of hot sorbent in the kiln. A very few temperature traces exhibited irregular or unusual behavior that could not be fit properly by the general function, and these fit parameters were also rejected.

Consider again Figure 7.4 that shows the bulk heating time constant, \( \tau \). The data clearly show a strong trend of increasing \( \tau \) as fill fraction increases. This trend is not unexpected, since the thermal time constant of the bed should increase as its volume to surface area ratio increases. There is no apparent trend associated with thermocouple location. There is also a trend of increasing \( \tau \) as the kiln rotation rate is decreased. This is not entirely surprising either, as the thermal time constant of the bed should increase as the heat transfer coefficient between the bed and kiln wall decreases. It has been observed by others that the kiln to bed heat transfer coefficient for a well-mixed bed does decrease as kiln rotation rate decreases (Lehmberg et al. 1977; Tscheng and Watkinson 1979).
The variation of the oscillation period $P$ is shown in Figure 7.5. It is readily seen that $P$ increases as fill fraction increases, and increases as rotation rate decreases. These trends also agree with the proposed source of these oscillations. The period $P$ should correspond to the time for a particle to travel around the bed and return to the same point, in other words, the rotation period of the bed. Clearly, as the kiln rotation rate decreases, the bed rotation period increases. As the fill fraction increases, the circumference of the bed also increases, causing the bed rotation period to increase. These expected trends are consistent with the data. In fact, the rotation period of the bed may be estimated from the fill fraction and kiln rotation rate. If one assumes that no slippage occurs between the bed and the kiln wall, and one assumes that the time for a particle to traverse the free surface of the bed is small, then the bed rotational period is the length of time a point on the kiln wall is covered by the bed. This is:
\[ P = \alpha_b / \omega_k \]  

(7.2)

\( P \) = the bed rotation period (seconds)

\( \omega_k \) = the kiln rotation rate (radians per second)

\( \alpha_b \) = the arc of the kiln wall covered by the bed (radians)

The \( \alpha_b \) term can be calculated from the fill fraction using the following formula:

\[ FF = \left( \alpha_b - \sin(\alpha_b) \right) / 2 \pi \]  

(7.3)

\[ FF = \left( \alpha_b - \sin(\alpha_b) \right) / 2 \pi \]

*Figure 7.5* Oscillation period \( P \) as a function of fill fraction, rotation rate, and thermocouple location.
Both the experimental and calculated values for $P$ are shown in Figure 7.6. Figure 7.7 shows the ratio, $P_{\text{experimental}} / P_{\text{calculated}}$. As can be seen from both of these figures, the calculated values are about 20% smaller than the experimental values, but the qualitative trends are in excellent agreement. Part of the discrepancy may be accounted for in the estimation of the bed fill fraction using weighed sorbent and a previously measured density. This sorbent density, measured in a beaker, may be greater than the sorbent density when it is loose in a moving bed, yielding fill fractions in the kiln somewhat larger than anticipated. The neglect of the time for particles to traverse the free surface of the bed may also account for some of the discrepancy. One may conclude that the rotational period of solids in a slumping or rolling bed may be predicted with reasonable accuracy in this relatively straightforward fashion.

Figure 7.6 Measured oscillation period and predicted bed rotational period as a function of fill fraction, rotation rate, and thermocouple location.
Figure 7.7 The ratio between measured and predicted bed rotational period $P$.

Figure 7.8 shows the variation of the oscillation decay constant $\theta$. The trend is very similar to that observed in Figure 7.5 for $P$, although the data show more scatter. One may postulate that the decay constant $\theta$ is proportional to the calculated bed rotational period $P$, and this is seen in Figure 7.9, where the only variation remaining is apparently noise. This relationship can be restated as follows: the rate of mixing in the bed is directly proportional to the rate at which solids are turned over in the bed. From Figure 7.9, the mean value of the ratio of $\theta / P$ is 1.78, with a standard error of 7.5%. This gives the following correlation:

$$\theta = 1.78 P_{\text{predicted}} \quad (7.4)$$
Figure 7.8 Decay constant $\theta$ as a function of fill fraction, rotation rate, and thermocouple location.

Figure 7.9 The ratio of decay constant $\theta$ to predicted bed rotational period $P$. 
Application of Results

The experimental data and the curve fitted parameters indicate that cold sorbent introduced onto hot sorbent in a rotary kiln does indeed undergo rapid heating due to mixing with the hot sorbent. This occurs in parallel with the bulk heating of all parts of the bed by the wall. Based on these observations, a simple model predicting the heating of the cold sorbent charge can be formulated as follows:

\[
T_{\text{charge}} = T_{\text{kiln}} + (T_{\text{cold}} - T_{\text{mix}}) \exp\left(-t/\theta\right) + (T_{\text{mix}} - T_{\text{kiln}}) \exp\left(-t/\tau\right) \tag{7.5}
\]

- \(T_{\text{charge}}\) = the time dependent temperature of the freshly charged material
- \(T_{\text{kiln}}\) = the steady temperature of the kiln walls
- \(T_{\text{cold}}\) = the initial temperature of the freshly charged material (ambient)
- \(T_{\text{mix}}\) = the unknown temperature that the cold and hot solids would come to after mixing in the absence of other heating

The proportions of cold and hot sorbent mixing at a particular axial location in the kiln are not entirely clear. The charge of cold sorbent in this study was loaded in a pile in the center of the bed to simulate the loading of a barrel of waste in an industrial system. Observations indicate that this raised pile of cold sorbent displaces hot sorbent in the bed along the kiln axis. This agrees with the fact that a thermocouple 15 cm from the center registered little or no temperature drop due to a charge of cold sorbent. It is also clear that the cold sorbent charge does not completely displace the hot sorbent, as evidenced by the oscillatory behavior of the temperature traces. Therefore, some quantity of hot sorbent remains to be mixed with the cold sorbent charge. Preliminary evidence indicates that the proportions of hot to cold sorbent at the charge location are approximately one to one. For this conceptual heat transfer model it will be assumed that the hot and cold sorbent mix in equal proportions, although further work is needed to test this assumption.
Without any external heating, this process will result in a mixture at the average temperature, $T_{mix}$, of the sorbent masses. Since the hot sorbent is initially at the kiln wall temperature and the cold sorbent is initially at ambient temperature, $T_{mix}$ will be the average of $T_{kiln}$ and $T_{cold}$. With these assumptions, the model of the temperature response of the cold sorbent becomes:

$$T_{charge} = T_{kiln} - 0.5 \left( T_{kiln} - T_{cold} \right) \left[ \exp\left( -t / \tau \right) + \exp\left( -t / \Theta \right) \right] \quad (7.6)$$

In this equation, $\Theta$ can be predicted using the preceding correlation directly from bed and kiln parameters, and $\tau$ can be predicted using a lumped thermal capacitance analysis similar to that used in previous bed models (Owens et al. 1991; Barr et al. 1989b). For the pilot scale kiln with a rotation rate of 1.0 rpm and a 5% fill fraction, one may predict the value of $\Theta$ to be 21.6 seconds and the value of $\tau$ to be 225 seconds. See Appendix C for the details of these calculations. Since $T_{cold}$ is 20°C and $T_{kiln}$ is 360°C in these experiments, the transient response of $T_{charge}$ can be predicted from equation (7.6).

The transient response of the bed when mixing between hot and cold charges is not accounted for is also calculated. Conceptually, this model assumes that a cold charge of solids enters the kiln on one end and axially displaces the hot solids. The cold and hot masses then do not mix because axial mixing is very slow. The cold solids do mix with themselves, allowing one to assume they are spatially isothermal as they heat up. These are the assumptions that are normally made for rotary kiln heat transfer models, where steady-state solids feed is assumed. The transient response of the charge in this case is calculated as:

$$T_{charge} = T_{kiln} - (T_{kiln} - T_{cold}) \exp\left(-t / \tau\right) \quad (7.7)$$
The results for $T_{\text{charge}}$ predicted by equations (7.6) and (7.7) are shown in Figure 7.10. Notice the very sharp initial rise in temperature due to mixing, followed by a much more gradual rise as the bed becomes well mixed. It is during this initial sharp rise in temperature that rapid waste evolution could occur. Notice how the isothermal bed prediction, which also uses a value of $t$ of 225 seconds, shows a much slower initial rise in temperature, even though both predictions eventually approach the kiln temperature.

**Figure 7.10** Predicted thermal response of a charge of fresh sorbent added to the kiln using the mixing model and using isothermal bed assumptions with no mixing.

**SUMMARY**

Previous work on the heating of solids in rotary kiln incinerators has focused on continuously fed solids where one may assume the bed is thermally uniform in the radial direction. For the first time, a pilot-scale kiln simulator was used to make experimental measurements of the temperature response of solids charged onto a preexisting hot bed. The temperature measurements yielded some indication of the mixing rate of the solids as
a function of kiln rotation rate and bed fill fraction, and clearly showed that initially the
bed is not thermally uniform. The data were fit to a function containing characteristic time
constants for the thermal heating and mixing process, and these time constants were
extracted. A simple model is used to correlate the mixing time constant with the rate at
which the bed turns over. This allows the thermal history of a charge of solids to be
predicted based upon measurable parameters of the kiln and bed. The predicted thermal
histories suggest that mixing greatly augments the initial rate of heat transfer to the fresh
charge of solids, and rapid evolution of volatile species could result. Much work remains
to be done to demonstrate that this approach can be applied to other systems operating
under different conditions. In particular, scaling of these results to field-scale rotary kilns
is of great importance. Further, this work does not predict the distribution of temperature
within the charge of solids, which may be necessary to predict accurately the evolution of
volatile species from the solids.
CHAPTER 8

CONCLUSIONS AND RECOMMENDATIONS

SUMMARY

Overall, this work has resulted in some important conclusions. Each chapter in this document has included the conclusions based upon that specific part of the work. For completeness, the major conclusions are summarized here.

A review of the literature presented in Chapter 2 reveals that there are very few published accounts of processes occurring within rotary kiln incinerators. There are a number of critical reviews on the general subject of incineration, but most publications deal with incinerator emissions as measured at the stack, with little or no mention of processes within the system. A number of studies, attributed solely to the group at LSU, document experimental measurements within a field-scale rotary kiln incinerator. A few other groups have presented experimental work using pilot-scale rotary kiln simulators to study specific phenomena that occur within rotary kilns, and these groups have also presented rudimentary models for predicting the evolution of volatile wastes from solids in these systems. Heat transfer within rotary kilns has been relatively well studied and documented; however, these studies have focused primarily on process rotary kilns and not rotary kiln incinerators. The regimes of bed motion exhibited by solids in rotary kilns have been well documented; however, the mixing of these solids is poorly characterized. Scaling analyses for rotary kiln design and performance are currently very crude. Empirical methods are used in the published accounts of rotary kiln design; however, detailed numerical modeling is proving itself as a powerful tool in the related area of coal-fired furnace design.
In Chapter 3, an experiment on a field-scale rotary kiln incinerator is described, and preliminary results including the O\textsubscript{2} response throughout the system are discussed. Combustion of the polyethylene packs alone was seen to have a negligible influence on the O\textsubscript{2} response. Considerable air leakage into the kiln was observed when the loading chute door was open. Vertical stratification at the kiln exit was observed, and was decreased with the addition of turbulence air. Observing the O\textsubscript{2} response in the kiln, afterburner, and stack for individual packs indicated that small perturbations in concentration persisted throughout the system, and were not lost due to axial mixing.

In Chapter 4, the experimental results are expanded upon. The use of ensemble averaged responses is shown to reduce the variation associated with individual packs, allowing easier comparison of the effects of independent variables. Gas chromatographic data is effectively used to support the continuous analyzer data. The bed motion in these experiments is observed to be in the slipping regime, which appears to reduce the influence of kiln rotation rate on the measured responses. Vertical stratification is observed in the O\textsubscript{2} concentration, CO\textsubscript{2} concentration, and gas temperature near the kiln exit plane. The upper kiln is characterized by lower O\textsubscript{2} concentration, higher CO\textsubscript{2} concentration, and higher gas temperatures. The addition of turbulence air appears to reduce the magnitude of stratification. Measured facility temperatures and measured gas temperatures do not agree well, probably because of radiation heat transfer from the facility thermocouples.

In Chapter 5, the ensemble averaged data are used to obtain information on air leak rates, toluene evolution rates, and to close mass balances on the toluene. Air leak rates into the system are calculated to be between 2.8 and 3.5 times the metered air flow rates. Cumulative toluene evolution rates are characterized by an exponential function, with an average time constant of 141 seconds. Good mass closure is obtained, which appears to be independent of the calculation method used. Overall, the mass balances and evolution time constants are independent of both kiln rotation rate and turbulence air
addition. This is attributed to the slipping bed motion observed during these experiments. Comparisons are made to earlier experiments of pack-loaded xylene incineration, where slumping bed motion was observed. The slipping motion was characterized by a single, large magnitude spike in contaminant evolution followed by a gradual decay to baseline. In contrast, the slumping motion was characterized by two or three maxima in evolution rate of smaller magnitude spread over a longer time. The results suggest that a slumping bed may be desirable for processing of solids contaminated with high concentrations of volatile wastes, while a slipping bed may allow greater throughput of low concentration waste or non-volatile contaminants.

In Chapter 6, a detailed, 3-dimensional numerical model of baseline operation in a rotary kiln incinerator is presented. The model is compared to experimental data and, although it is relatively crude, it demonstrates remarkably good qualitative and quantitative predictive capability. The model demonstrates that thermal buoyancy is indeed the cause of the observed vertical stratification near the kiln exit. The model also suggests that the addition of turbulence air actually increases the degree of stratification rather than augmenting mixing as had been suggested previously. By elucidating the mechanism by which this occurs, the model has demonstrated its utility and resulted in a reinterpretation of the experimental data. The model suggests that there is probably a zone of recirculation across the kiln exit plane. A parametric study using the model suggests that the location and quantity of leak air have a major influence on the flow in the kiln. The study also suggests that preheating turbulence air may have little effect on gas-phase mixing. Overall, this modeling study has demonstrated that a relatively simple numerical model of a rotary kiln incinerator can provide valuable insight into the process, especially when used in conjunction with experimental data.

In Chapter 7, a study of solids mixing in the bed of a rotary kiln is presented. The study uses a pilot-scale rotary kiln for experimental measurement of solids mixing rates as determined by their temperature. The temperature data is curve fit and the results
demonstrate that the mixing rate is directly proportional to the rate of solids circulation through the bed. The proportionality constant is empirically determined, however the rate of solids circulation through the bed can be predicted theoretically. The result is a predictive model for solids mixing in a rotary kiln, and the utility of this result is demonstrated by an example. The mixing of solids in the bed of a rotary kiln is concluded to be of major importance in determining its thermal history and ultimately the rate of contaminant evolution from the bed.

RECOMMENDATIONS FOR FURTHER WORK

The research presented in this document represents substantial progress toward the goal of understanding rotary kiln incinerators and developing predictive capability for these systems. However, it is clear that much work remains to be done toward these goals. The following is a list of specific recommendations of what work needs to be done, based upon the results obtained in this current work.

(1) The toluene test matrix used in this work needs to be repeated without a bed thermocouple, and with visual verification that slumping motion occurs. The toluene evolution rates should be calculated using only the stack O₂ response to simplify the experiment. This evolution data should be used for comparisons with the current slipping motion data and for scaling purposes.

(2) With good field-scale results from the same bed motion regime [from (1)], an improved scaling model for contaminant evolution needs to be developed. This may require additional pilot-scale experiments for verification.

(3) Using a more manageable probe with velocity-measurement capabilities, the kiln exit plane velocity field, temperature field, and concentration field should be measured. This test is needed to obtain a map of conditions over the entire kiln
exit plane, not just at two points. This data will be extremely useful for detailed numerical model verification.

(4) Preliminary tests to determine the influence of pack size and composition on evolution rate are needed. Again, the evolution rate should be calculated using only the stack \( O_2 \) response to simplify the experiment. If a packaging means can be found that reduces the peak evolution rates, the potential benefit to the industry may be tremendous.

(5) This study has focused on a single field-scale rotary kiln incinerator designed a number of years ago. A survey of rotary kiln manufacturers is needed to determine what design features are being implemented today, what features are common among most modern rotary kiln incinerators, and what innovative features are available. This is needed to address the ongoing applicability of this work, and to begin to generalize the results to incinerators other than the one studied in detail.

(6) The detailed 3-D numerical model of a rotary kiln incinerator should be refined. A finer grid needs to be implemented, and radiation heat transfer must be included in the formulation. Together with a detailed experimental map of the kiln exit plane, this model may be verified and used to elucidate finer features of the flow in the kiln, in particular the sources and influence of leak air.

(7) A preliminary transient numerical model needs to be formulated to address the influence of contaminant evolution and combustion on the flow and temperature field. Initially, to make the problem tractable, this model should retain a coarse grid and neglect radiation heat transfer. As software and hardware improve, it may be refined as in (6) to produce a very powerful and realistic model. This model should yield substantial insight into the dynamics of pack combustion in a rotary kiln incinerator.
The empirical model of solids mixing in a rotary kiln needs to be expanded. In particular, the influence of particle size and shape, and the appropriate scaling parameters, should be determined. The effect of initial charge distribution on the mixing process needs to be addressed. Similar data from a different-sized kiln needs to be obtained to verify the general applicability of the empirical model and the scaling parameters. Finally, this mixing model should be incorporated into heat and mass transfer models of the contaminated bed to provide more realistic predictive capability for contaminant evolution.
BIBLIOGRAPHY


APPENDIX A

LISTING OF THE NUMERICAL MODEL SPECIFICATIONS

TA-OFF BASELINE CASE

******************************************************************************
* *
* FLUENT (V3.03) Fluid Flow Modeling *
* *
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* Etna Road, PO Box A-219 *
* Hanover, New Hampshire 03755 USA *
* (800) 445-4454 *
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16 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & 16 \\
15 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & 15 \\
14 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & 14 \\
13 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & 13 \\
12 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & 12 \\
11 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & 11 \\
10 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & 10 \\
9 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & 9 \\
8 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & 8 \\
7 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & 7 \\
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3 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & 3 \\
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1 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & 1 \\
\end{array}
\]

\( K = 4 \) THROUGH \( K = 28 \) ARE IDENTICAL TO \( K = 3 \)

\( K = 29 \)

\[
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12 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & 12 \\
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9 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & 9 \\
8 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & 8 \\
7 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & 7 \\
6 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & 6 \\
5 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & 5 \\
4 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & 4 \\
3 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & 3 \\
2 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & 2 \\
1 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & W1 & 1 \\
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**K = 31 THROUGH K = 35 ARE IDENTICAL TO K = 30**

**K = 36**

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<th>J</th>
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| J | I= | 2 | 4 | 6 | 8 | 10 | 12 | 14 | 16 | -I | J |
- CHEMICAL SPECIES DEFINITIONS -

TOTAL NUMBER OF CHEMICAL SPECIES = 6
NUMBER OF GAS PHASE SPECIES = 6
NUMBER OF SURFACE SPECIES = 0
NUMBER OF SPECIES EQUATIONS SOLVED = 5

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- REACTION STOICHIOMETRY DEFINITION -

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<td>H2O</td>
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- REACTION RATE CONSTANTS -

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### Velocity/Turbulence Boundary Conditions

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### Chemical Species Boundary Conditions

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</table>

### Gravitational Accelerations

\[
x = 0.0000E+00 \\
y = -9.8100E+00 \\
z = 0.0000E+00
\]
- TURBULENCE MODEL CONSTANTS -

\[
\begin{align*}
C_D &= 5.5 \times 10^{-1} \\
C_1 &= 1.4 \times 10^0 \\
C_2 &= 1.9 \times 10^0 \\
\text{MU} &= 9.0 \times 10^{-2} \\
R\text{SMCD} &= 1.0 \times 10^0
\end{align*}
\]

- WALL FUNCTION TURBULENCE MODEL CONSTANTS -

<table>
<thead>
<tr>
<th>WALL ZONE</th>
<th>Cappa</th>
<th>ELOG</th>
</tr>
</thead>
<tbody>
<tr>
<td>W1</td>
<td>4.187 \times 10^{-1}</td>
<td>9.793 \times 10^0</td>
</tr>
<tr>
<td>W2</td>
<td>4.187 \times 10^{-1}</td>
<td>9.793 \times 10^0</td>
</tr>
<tr>
<td>W3</td>
<td>4.187 \times 10^{-1}</td>
<td>9.793 \times 10^0</td>
</tr>
</tbody>
</table>

- USER DEFINED PHYSICAL MODELS -

NON-NEWTONIAN FLUID - NO

- USER DEFINED PROPERTIES -

FLUID VISCOSITY - NO
FLUID DENSITY - NO
FLUID SPECIFIC HEAT - NO
FLUID THERMAL CONDUCTIVITY - NO
TURBULENT VISCOSITY - NO

- USER DEFINED SOURCE TERMS -

X-MOMENTUM EQUATION - NO
Y-MOMENTUM EQUATION - NO
Z-MOMENTUM EQUATION - NO
PRESSURE CORRECTION EQUATION - NO
TURBENT K.E. EQUATION - NO
TURB. K.E. DISSIPATION EQUATION - NO
ENTHALPY EQUATION - NO
SPECIES EQUATIONS - NO

- USER STARTUP SUBROUTINE IS NOT ACTIVE -

- USER DEFINED ADJUSTMENTS -

X-MOMENTUM EQUATION - NO
X-MOMENTUM EQUATION - NO
X-MOMENTUM EQUATION - NO
X-MOMENTUM EQUATION - NO
- PROPERTY CALCULATION OPTIONS -

COMPOSITION DEPENDENT VISCOSITY - NO
COMPOSITION DEPENDENT THERMAL CONDUCTIVITY - NO
COMPOSITION DEPENDENT SPECIFIC HEAT - YES
ANY PROPERTY COMPUTED USING KINETIC THEORY - NO
ENABLE USER SPECIFIED MIXING LAWS - NO

- DENSITY IS COMPUTED FROM THE IDEAL GAS LAW
- THE OPERATING PRESSURE = 1.0133E+05

- SPECIES MOLECULAR WeIGHTS -

<table>
<thead>
<tr>
<th>SPECIES NAME</th>
<th>MOLECULAR WEIGHT</th>
</tr>
</thead>
<tbody>
<tr>
<td>N2</td>
<td>2.8000E+01</td>
</tr>
<tr>
<td>O2</td>
<td>3.2000E+01</td>
</tr>
<tr>
<td>CH4</td>
<td>1.6000E+01</td>
</tr>
<tr>
<td>CO2</td>
<td>4.4000E+01</td>
</tr>
<tr>
<td>H2O</td>
<td>1.8000E+01</td>
</tr>
<tr>
<td>INERT</td>
<td>2.8000E+01</td>
</tr>
</tbody>
</table>

- MIXTURE VISCOSITY DEFINITION -

VISC. = 4.204E-06 + 5.555E-08*T**1 - 2.518E-11*T**2 + 9.074E-15*T**3 - 1.160E-18*T**4

- SPECIFIC HEAT DEFINITION -

SPECIFIC HEAT FOR N2
CP = 9.755E+02 + 1.869E+01*T**1 - 1.495E-07*T**2

SPECIFIC HEAT FOR O2
CP = 8.044E+02 + 4.059E+01*T**1 - 1.208E-04*T**2

SPECIFIC HEAT FOR CH4
CP = 8.847E+02 + 4.722E+01*T**1 - 1.125E-03*T**2

SPECIFIC HEAT FOR CO2
CP = 5.913E+01 + 9.892E+01*T**1 - 3.373E-04*T**2

SPECIFIC HEAT FOR H2O
CP = 1.688E+03 + 5.345E+01*T**1 + 6.583E-05*T**2

SPECIFIC HEAT FOR INERT
CP = 9.755E+02 + 1.869E+01*T**1 - 1.495E-07*T**2

ENTHALPY REFERENCE TEMPERATURE = 2.9800E+02

- MIXTURE THERMAL CONDUCTIVITY DEFINITION -

K = 3.089E-02 - 6.055E-05*T**1 + 2.046E-07*T**2 - 1.342E-10*T**3 + 2.984E-14*T**4

- FORMATION ENTHALPY INFORMATION -

<table>
<thead>
<tr>
<th>SPECIES NAME</th>
<th>FORMATION ENTHALPY</th>
<th>REFERENCE TEMPERATURE</th>
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</thead>
<tbody>
<tr>
<td>N2</td>
<td>0.0000E+00</td>
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<tr>
<td>O2</td>
<td>0.0000E+00</td>
<td>2.9800E+02</td>
</tr>
<tr>
<td>CH4</td>
<td>-7.4873E+07</td>
<td>2.9800E+02</td>
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<tr>
<td>CO2</td>
<td>-3.9352E+08</td>
<td>2.9800E+02</td>
</tr>
<tr>
<td>H2O</td>
<td>-2.4183E+08</td>
<td>2.9800E+02</td>
</tr>
<tr>
<td>INERT</td>
<td>0.0000E+00</td>
<td>2.9800E+02</td>
</tr>
</tbody>
</table>
- Solution Control Parameters -

SOLVER MARCHING DIR. = Y-DIRECTION
SOLVER SWEEP DIR. = Z-DIRECTION
ALTERNATE SWEEP DIR. = NO
SOLVER ACCEL. FACTOR = 1.00
SOLUTION METHOD = SIMPLEC
PATCH OPTION = NO
CONVERG/DIVERG CHECK = NO
NORMALIZE RESIDS. = YES
CONTINUITY CHECK = YES
RESET OPTION = YES
REYNOLDS STRESS MODEL = YES
MONITOR SOLVER = NO
COMPRESSIBLE FLOW = NO
COMP./VAR. VIS. TERMS = NO
VISCOSOUS DISSIPATION = NO
BLOCK CORRECTION = YES

SECOND RELAXATION FACTORS ON AFTER 32000 ITERATIONS

DIFFERENCING SCHEME = QUADRATIC UPWIND (QUICK)

REFERENCE PRESSURE LOCATION:

I = 8
J = 2
K = 2

<table>
<thead>
<tr>
<th>VARIABLE</th>
<th>SOLVED</th>
<th>NO. SWEEPS</th>
<th>UNDERRELAX 1</th>
<th>UNDERRELAX 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>PRESSURE</td>
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<td>6.0000E-01</td>
<td>5.0000E-02</td>
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<td>3.0000E-01</td>
<td>2.0000E-02</td>
</tr>
<tr>
<td>V-VELOCITY</td>
<td>YES</td>
<td>8</td>
<td>3.0000E-01</td>
<td>2.0000E-02</td>
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<tr>
<td>W-VELOCITY</td>
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<td>3.0000E-01</td>
<td>2.0000E-02</td>
</tr>
<tr>
<td>TURB. K.E.</td>
<td>YES</td>
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<td>3.0000E-01</td>
<td>2.0000E-02</td>
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<tr>
<td>K.E. DISS.</td>
<td>YES</td>
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<td>3.0000E-01</td>
<td>2.0000E-02</td>
</tr>
<tr>
<td>ENTHALPY</td>
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<td>6.0000E-01</td>
<td>2.0000E-02</td>
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<tr>
<td>BLOCK COR.</td>
<td>YES</td>
<td>N/A</td>
<td>6.0000E-01</td>
<td>3.0000E-01</td>
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<td>N2</td>
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<td>2.0000E-02</td>
</tr>
<tr>
<td>O2</td>
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<td>6.0000E-01</td>
<td>2.0000E-02</td>
</tr>
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<td>6.0000E-01</td>
<td>2.0000E-02</td>
</tr>
<tr>
<td>CO2</td>
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<td>6.0000E-01</td>
<td>2.0000E-02</td>
</tr>
<tr>
<td>H2O</td>
<td>YES</td>
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<td>6.0000E-01</td>
<td>2.0000E-02</td>
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<td>PROPERTIES</td>
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<td>N/A</td>
<td>N/A</td>
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<tr>
<td>VISCOSITY</td>
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<td>N/A</td>
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<td>2.0000E-02</td>
</tr>
<tr>
<td>TEMPERATURE</td>
<td>N/A</td>
<td>N/A</td>
<td>6.0000E-01</td>
<td>3.0000E-02</td>
</tr>
</tbody>
</table>

- Time Dependence -

TIME STEP LENGTH (SECONDS) = 2.50000E-01
MAXIMUM NUMBER OF ITERATIONS PER STEP = 20
MINIMUM RESIDUAL SUM (TO TRIP STEP) = 1.000E-03
MINIMUM ENTHALPY RESIDUAL (TO TRIP STEP) = 1.000E-06
AUTO SAVE = NO
TA-ON BASELINE CASE

Only the differences in model specifications are listed. All other specifications are identical to the TA-off Baseline Case.

- VELOCITY/TURBULENCE BOUNDARY CONDITIONS -

<table>
<thead>
<tr>
<th>ZONE</th>
<th>U-VELOCITY</th>
<th>V-VELOCITY</th>
<th>W-VELOCITY</th>
<th>TURB. K.E.</th>
<th>K.E. DISSIP.</th>
</tr>
</thead>
<tbody>
<tr>
<td>W1</td>
<td>0.0000E+00</td>
<td>0.0000E+00</td>
<td>0.0000E+00</td>
<td>SET</td>
<td>SET</td>
</tr>
<tr>
<td>W2</td>
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<td>0.0000E+00</td>
<td>SET</td>
<td>SET</td>
</tr>
<tr>
<td>W3</td>
<td>0.0000E+00</td>
<td>0.0000E+00</td>
<td>0.0000E+00</td>
<td>SET</td>
<td>SET</td>
</tr>
<tr>
<td>I1</td>
<td>-1.4826E+00</td>
<td>-5.4203E-01</td>
<td>7.7703E+00</td>
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<td>I2</td>
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<td>1.1165E+01</td>
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<tr>
<td>I3</td>
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<td>1.0264E+00</td>
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<td>0.0000E+00</td>
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<td>1.9100E+05</td>
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<tr>
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<td>0.0000E+00</td>
<td>8.7357E-01</td>
<td>1.1447E-04</td>
<td>4.0446E+06</td>
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<tr>
<td>I6</td>
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<td>2.1343E-01</td>
<td>0.0000E+00</td>
<td>6.8328E-06</td>
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<td>0.0000E+00</td>
<td>1.1232E+00</td>
<td>1.8922E-04</td>
<td>3.1667E-05</td>
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<td>I8</td>
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<td>1.3289E+00</td>
<td>8.2692E+00</td>
<td>1.2066E+00</td>
<td>2.6262E+01</td>
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<tr>
<td>I9</td>
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<td>2.6984E+00</td>
<td>8.2692E+00</td>
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<td>IA</td>
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<td>0.0000E+00</td>
<td>2.4553E-01</td>
<td>9.0425E-06</td>
<td>5.3800E-07</td>
</tr>
</tbody>
</table>

- CHEMICAL SPECIES BOUNDARY CONDITIONS -

<table>
<thead>
<tr>
<th>ZONE</th>
<th>N2</th>
<th>O2</th>
<th>CH4</th>
<th>CO2</th>
<th>H2O</th>
</tr>
</thead>
<tbody>
<tr>
<td>W1</td>
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<td>LINK CUT</td>
<td>LINK CUT</td>
<td>LINK CUT</td>
<td>LINK CUT</td>
</tr>
<tr>
<td>W2</td>
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<td>LINK CUT</td>
<td>LINK CUT</td>
<td>LINK CUT</td>
<td>LINK CUT</td>
</tr>
<tr>
<td>W3</td>
<td>LINK CUT</td>
<td>LINK CUT</td>
<td>LINK CUT</td>
<td>LINK CUT</td>
<td>LINK CUT</td>
</tr>
<tr>
<td>I1</td>
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<td>0.0000E+00</td>
</tr>
<tr>
<td>I5</td>
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<td>0.0000E+00</td>
<td>0.0000E+00</td>
</tr>
<tr>
<td>I6</td>
<td>7.6915E-01</td>
<td>2.3085E-01</td>
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<td>0.0000E+00</td>
<td>0.0000E+00</td>
</tr>
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</tbody>
</table>

- TEMPERATURE BOUNDARY CONDITIONS -

<table>
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<th>ZONE</th>
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</tr>
</thead>
<tbody>
<tr>
<td>W1</td>
<td>8.0000E+02</td>
</tr>
<tr>
<td>W2</td>
<td>8.0000E+02</td>
</tr>
<tr>
<td>W3</td>
<td>4.0000E+02</td>
</tr>
<tr>
<td>I1</td>
<td>3.0729E+02</td>
</tr>
<tr>
<td>I2</td>
<td>3.0600E+02</td>
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<td>I3</td>
<td>3.0692E+02</td>
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<tr>
<td>I4</td>
<td>3.1000E+02</td>
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<tr>
<td>I6</td>
<td>3.1000E+02</td>
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</tbody>
</table>
The time constant $\theta$, used to describe the decay of the temperature oscillation, is the result of a combination of effects. The difference in temperature between the hot and cold sorbent masses is reduced by conduction through the bed over a length of approximately one bed thickness, and by physical mixing of the sorbent followed by heat conduction between particles over a length of approximately one particle diameter. Since the proposed conceptual model does not delineate these two effects, this difference is not important to the model implementation. However, the importance of physical mixing as opposed to static heat conduction can be demonstrated. The measured sorbent thermal conductivity, $k$, specific heat, $c_p$, and density, $\rho$, are (Owens et al. 1991):

\begin{align*}
  k &= 0.174 \text{ W/m-K} \\
  c_p &= 1000 \text{ J/kg-K} \\
  \rho &= 650 \text{ kg/m}^3
\end{align*}

Assume that equal charges of cold and hot sorbent are brought together with no mixing in two layers evenly distributed in the bottom of the kiln. Further assume this is done at the 3% fill fraction, yielding an approximate bed thickness of 2.6 cm. Assume, for demonstration purposes, that this situation can be approximated by a slab geometry and that the boundaries are insulated; that is there is no heat exchange with the kiln. This problem is summarized in Figure B.1.
The governing equation for the temperature of the bed is the one-dimensional transient heat conduction equation. Due to symmetry, the boundary condition at the interface between the hot and cold parts of the bed is the average of the initial hot and cold bed temperatures, \( T_{\text{ave}} \). The transient response of the temperature at the upper edge of the cold bed \( (x = L/2) \) given by Carslaw and Jaeger (1959) is:

\[
\frac{T - T_{\text{ave}}}{T_{\text{cold}} - T_{\text{ave}}} = \frac{4}{\pi} \sum_{n=0}^{\infty} \frac{1}{(2n+1)} \exp \left[ \frac{-\alpha(2n+1)^2}{L^2} \right] \sin \left[ \frac{(2n+1)\pi x}{L} \right]
\]  

(B.1)
For relatively large times, the solution can be approximated as the first term of the series. In this case, the characteristic time for a point at \( x = L/2 \) is:

\[
\tau = \frac{L^2}{(\alpha \pi^2)} \quad \text{(B.2)}
\]

Using the bed parameters given above, \( \tau \) is 262 seconds. For this value of time the one-term approximation is very good. This characteristic time is larger than any decay constant, \( \theta \), measured experimentally. In fact, for rotation rates of 0.4 rpm and higher, the characteristic bed conduction time is at least an order of magnitude greater than the measured decay time constant. This would imply that the observed decay in temperature fluctuations is due almost entirely to particle mixing. At very slow rotation rates the bed conduction characteristic time and the observed decay time constant become of the same order of magnitude, and conduction through the bed may contribute significantly to the decay of the temperature fluctuations.
APPENDIX C

SAMPLE CALCULATION FOR THERMAL TIME CONSTANTS

The following calculations provide time constants $\theta$ and $\tau$ for use in equations (7.6) and (7.7), with the results graphed in Figure 7.10.

1. Given parameters and definition of variables.

   $R = \text{kiln radius} = 0.305 \text{ m}$
   $n = \text{kiln rotation rate} = 1/60 \text{ revolutions/second}$
   $FF = \text{kiln fill fraction} = 0.05$
   $\rho, k, c$ are properties of the sorbent, given in Appendix A.
   $\alpha$ is the sorbent thermal diffusivity $= k/\rho c$
   $\alpha_b$ is the central angle of the kiln occupied by the bed, in radians

2. Calculation of central angle occupied by the bed, $\alpha_b$, from equation (7.3).

   $FF = ( \alpha_b - \sin(\alpha_b) ) / 2 \pi$
   For given fill fraction, solve iteratively for $\alpha_b$. Result is 1.269 rad.

3. Calculation of bed rotational period, $P$, from equation (7.2).

   $P = \frac{\alpha_b}{\omega_k}$
   $P = 1.269 \text{ rad} / ((1/60 \text{ revolutions/sec}) \times 2\pi \text{ rad/revolution})$
   $P = 12.118 \text{ sec}$
4. Calculation of mixing time constant, $\theta$, from equation (7.4).

\[
\theta = 1.78 \, P_{\text{predicted}} \\
\theta = 1.78 \times 12.118 \, \text{sec} \\
\theta = 21.57 \, \text{sec}
\]

5. Estimation of heat transfer coefficient between wall and bed solids, $h_{ws}$.

From Tscheng and Watkinson (1979), a simple penetration theory model is used.

\[
h_{ws} = 2 \, k \left( \frac{2 \, n}{\alpha \, \alpha_p} \right)^{0.5}
\]

\[
\alpha = \frac{(0.174 \, \text{W/m K})}{((650 \, \text{kg/m}^3) \times (1000 \, \text{J/kg K}))} = 2.677 \times 10^{-7} \, \text{m}^2/\text{s}
\]

\[
h_{ws} = 2 \times 0.174 \times \left( \frac{(2 \times 1)}{(60)} \right) \times \left( \frac{2.677 \times 10^{-7} \times 1.269}{0.5} \right)
\]

\[
h_{ws} = 109 \, \text{W/m}^2\text{K}
\]

6. Estimation of the bulk thermal time constant, $\tau$, using lumped thermal capacitance.

\[
\tau = \frac{(\rho \, V \, c)}{(h \, A)}
\]

Where $V$ is the volume of the bed and $A$ is the area contacting the kiln wall.

Assuming a kiln of unit length,

\[
V = FF \times \pi \times R^2
\]

\[
A = R \times \alpha_p
\]

\[
\tau = \frac{(650 \times 0.05 \times \pi \times 0.305^2 \times 1000)}{(109 \times 0.305 \times 1.26895)}
\]

\[
\tau = 225 \, \text{seconds}
\]
VITA

Christopher Brian Leger was born on January 3, 1965 in Houston, Texas. As a child, he was always fascinated by fire. He moved with his family to Crowley, Louisiana in 1980 and graduated from high school there in 1983. He entered Louisiana State University in August, 1983, majoring in mechanical engineering. As a sophomore, he got a job as a student worker in the Incineration Laboratory under Dr. Vic Cundy. Upon graduation with a B.S. in Mechanical Engineering in May, 1987, he received a National Science Foundation fellowship and decided to pursue his Ph.D in the Incineration Laboratory at LSU. His time spent in graduate school at LSU has been both educational and rewarding. The opportunities to travel to Germany and Utah in the course of his research have been particularly enjoyable. Although the author has specialized in combustion and has learned much about the phenomenon, he is still fascinated by fire.
DOCTORAL EXAMINATION AND DISSERTATION REPORT

Candidate: Christopher Brian Leger

Major Field: Mechanical Engineering

Title of Dissertation: A Study of Selected Phenomena Observed During Rotary Kiln Incineration

Approved:

[Signature]
Major Professor and Chairman

[Signature]
Dean of the Graduate School

EXAMINING COMMITTEE:

[Signature]

[Signature]

[Signature]

Edward B. Overton

Date of Examination:

July 14, 1992