# Konvertering av högtemperaturugnar från olja och gasol till naturgas

- Verkningsgrad
- Kapacitet
- NOx-bildning





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#### ABSTRACT

This report aims at clarifying the questions raised by an industrial furnace or boiler user currently using fuel-oil or LPG and considering switching to natural gas. The issues of changes of performance and pollutant emission are addressed. These are accomplished by a two-fold study: a literature survey and discussion of nitrous oxides formation; a study from first principles supported by a literature survey of a radiative enclosure analysis relevant to furnace and boiler applications. The latter presentation aims at clarifying the differences between a mixture composed of spectral gases and soot, and a mixture of only spectral gases.

A main question being asked is: Can the strongly spectral products of combustion of natural gas be analyzed without recourse to full spectral radiation analysis? The answer being "yes," a simplified model is developed and validated by comparison to results found in the literature. Some illustrative cases are presented and a program manual is included. Typically, the program takes on the order of a few minutes to run on a desk-top computer. The program is intended for industrial furnace and boiler owners to use as a preliminary assessment of performance changes if they were to switch from their current fuel to natural gas.

Rapporten är beställd av Mats Johansson, Swedegas, och ingår i Swedegas FUD-program för 1988.

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#### CHAPTER 1: GENERAL CONSIDERATIONS

In the way of introduction and for the sake of completion we will present many features of natural gas which make it a very attractive and competitive fuel in today's market. The stage has been set for the widespread use of natural gas, amongst other reasons, by:

- the steady increasing price of fossil fuels;
- the attempt of governments to diversify their energy sources;
- the emphasis of society on pollution reduction; and
- the deemphasis on nuclear power.

This conjuncture opened the stage for new fuel alternatives. Natural gas has become a prime candidate in Europe, and Scandinavia specifically, because:

- vast reserves of the fuel from various countries have been discovered, Ruhrgas Aktiengesellschaft (1984)\$;
- it is considered a "clean fuel;"
- it is considered a versatile fuel for stationary applications; and
- experience for its widespread use can be gathered from the USA and more recently, late 1960s, from England, see British Gas (1988).

A range of industrial applications have been cited for natural gas, Chaignon and Breney (1987) and Svenska Gasföreningen (1986). Particular advantages of this fuel are:

S All references are listed in REFERENCES 1 by author (year); references relating specifically to NO<sub>x</sub>, Chapter 2, are listed in REFERENCES 2.

- contains no fuel bound mitrogen, therefore no fuel-NO<sub>x</sub> is produced;
- has low sulfur content;

- possesses good mixing characteristics resulting in low air consumption, which in turn results in reduced fan power and in reduced ND<sub>4</sub> emissions;
- delivers even radiative flux to load--radiation not concentrated in flame;
- low concentration of soot and suspended solids means low maintenance costs, elimination of filtering/solids recovery equipment, etc; and
- where applicable, refractory lining life is extended because of the low sulfur content.

It is only natural that with the potential supply of the gas fields in the Netherlands, Denmark, Norway, and the availability of Soviet natural gas, the interest in the conversion and optimization of old oil-fired units and the introduction of new single and dualfuel furnaces is on the agenda. The conversion of oil-fired furnaces and boilers to natural gas firing has been covered relatively well in the literature. In Europe, this has occurred due to the introduction of natural gas, for example, in Britain in the 1960s'. As a result much theoretical work was done in the late 60s' and early 70s' in this area: Midlands Research Station, owned by British Gas, the International Flame Research Foundation, in the Netherlands, and others in the United States, Germany, and more recently in Japan have contributed for clarifying the differences between the two fuels.

We will concern ourselves in this paper with the technical aspects of fuel performance as far as heat transfer and furnace performance. The rather interesting economic, environmental, and geopolitical aspects, which are a must for a complete comparison of the two fuels, will not be covered. From these nontechnical concerns alone indicate natural gas is indeed a good alternative to fuel-oil.

From the point of view of the furnace owner though, the question of thermal performance arises and will be addressed in this paper.

The important differences in performance relate to the impact on furnace efficiency and on furnace capacity. These concerns naturally arise because, firstly, it is known that the radiation emitted by a luminous flame, e.g., that of heavy oil, is higher than that emitted by a nonluminous one, e.g., that of natural gas; secondly, much operating experience has been accumulated on fuel-oil furnace operation. It must be clearly explained to the furnace owner that a performance comparison of the two fuels is inadequate if kept only to this "visible" difference. It is important to point out that the flame is only one part of the total combustion/heat transfer environment in the furnace chamber.

A comparison of the two fuels, then, must address the following differences:

- 1. Luminous versus nonluminous flames;
- 2. Spectral characteristics of the products of combustion;
- 3. Partial pressures of radiating gases;
- 4. Excess air requirements;
- 5. Flame temperatures; and
- 6. Impact of convection and wall radiation.

These items will be addressed in this report. In accordance with Swedegas AB, the goals of the project are:

- Treatment of NO<sub>x</sub> formation during the combustion of natural gas and oil, and to a smaller extent of propane. This will include a literature survey and a discussion of published and unpublished findings in this area.
- 2. Development of the theoretical differences between natural gas-fired and oil-fired industrial furnaces in the areas of ...

capacity, efficiency, and related topics. This discussion will include a literature search of relevant material and dwell specifically on the radiative modeling of one fuel versus another and take special account of the treatment of the spectral radiative differences between them. In this light, it will cover luminous versus nonluminous flames.

3. Delivery of a user-friendly mathematical model to Swedegas which can be easily run on a personal computer. This model will cover an industrial furnace or boiler of simple geometry; it will account in a simple but accurate manner for the effects of spectral radiation in the furnace; within certain bounds, the user can specify the geometry, the fuel type, and some operating conditions as to enable the performance comparison between one fuel and another. Some validation of this model by comparison with published data will be made.

This report is organized as follows. Chapter 2 covers the literature and discusses the formation of nitrous oxides in combustion. The references for this chapter are listed separately from all others for clarity in References 2. Chapter 3 covers furnace modeling and associated review of the literature. Chapter 4 details the development of the model and its validation and application.

#### CHAPTER 2: NOL FORMATION

#### 2.1 BACKGROUND

The generic symbolism represented by the term nitrous oxides, NO<sub>4</sub>, refers to a whole group of N=O compounds, mostly ND and NO<sub>4</sub>, but also NO<sub>1</sub>, N<sub>2</sub>O, N<sub>4</sub>O<sub>4</sub>, N<sub>2</sub>O<sub>4</sub>. During a combustion process, in the presence of relatively high temperatures atomic, nitrogen is combined with atomic oxygen to form for the most part nitrogen monoxide, NO--about 90% of all nitrous oxides formed. Eventually this gas is further oxidized to NO<sub>4</sub> by residual oxidants in the flue gas (or in a sampling probe!) and after discharge into the atmosphere.

The sources of NO. can usually be traced to the combustion of some fossil fuel. With the more intense exploitation of other alternate fuels, such as biomass, we can expect an increased contribution from them too. The sources can also be categorized as stationary or as mobile. Examples of stationary sources of nitrous oxides are power plants, industrial plants, and we cannot forget other sources such as the indoor polluters like the unvented space heater. The automobile is the typical example of a mobile source. The automobile emits the most nitrous oxides followed by utility power boilers, Nutcher (1984).

It is not a doubt anymore that nitrous oxides are serious pollutants. Typically, NO from combustion reacts with atomic oxygen in the atmosphere to produce  $NO_2$ .  $NO_2$  can then undergo photochemical decomposition to atomic and molecular oxygen which will eventually form ozone,  $O_3$ . The problems resulting from ozone in the atmosphere are now considered very important. But on a more visible and pressing scale, the ozone reacts with unburned hydrocarbons, especially those unsaturated, forming multiple bonds with the carbon. The resulting mess is known as 'smog.' Smog, of course, reduces visibility,

irritates the eyes and the respiratory organs, and causes forest damage.

As a result, regulations have been put into effect by governmental bodies to ameliorate the situation. Dacey (1985), for example, gives some figures for these environmentally acceptable limits from stationary sources:

	(40x (mg/m²)			
Country-year	Coal	oil	Natural Ga	5
USA-78	737	460	318	
Euro. Comm75	8007400	450/220	350/180	

In some problem areas such as in New York City, special laws have been promulgated. For example in 1971: 150 ppm for oil and 130 ppm natural gas, at 10% air, became the adopted emission limits.

#### 2.2 CHEMICAL/KINETIC ASPECTS OF NO, FORMATION

Because NO<sub>1</sub> is made of nitrogen and oxygen atoms, it is obvious that to start with we need both elements present in the combustion zone. Nitrous oxide formation can then be classified as to the source of the nitrogen atoms:

Molecular N  $(N_e)$ : Air-ND N chemically bound to fuel  $(C_x H_y N)$ : Fuel-ND

2.2.1 Air-NO

Unbound mitrogen can combine with oxygen through two main mechanisms: thermal-NO and prompt-NO. In thermal-NO the factors of major influence are: the flame temperature, the oxygen availability, and the residence time in the combustion region. Prompt-NO is basically the name given to the reactions not described by the Zeldovich Mechanism of thermal-NO. Early in the flame front, and by a process still not well understood, where O concentration is low, a small amount of NO was experimentally measured to be formed. Fenimore (1971). In this region, classical formation reactions are too slow to predict any NO formation. The process is believed to involve reactions of N<sub>2</sub> with fuel fragments mainly through, Careto (1976),

 $CH + N_2 \langle -- \rangle HCN + N$ 

The cyanide intermediate, through reactions akin to those of fuel-NO, results in NO:

N + OH (---> NO + H

Prompt-NO forms well down stream of the flame and at temperatures below 1300°C so it is not very temperature dependent as opposed to thermal-ND which is discussed next.

Thermal-NO is formed as a result of high-temperatures and so it is strongly temperature-dependent. Downstream from the flame, NO formation is well correlated by the classical reactions of Zeldovich and Semenov (1949):

 $N_e + 0 \langle --- \rangle NO + N$  (rate determining step)  $N + O_e \langle --- \rangle NO + O$  $N_e + O_e \langle --- \rangle 2NO$ 

Notice the chain mechanism of the two above reactions: the flame provides two conditions for NO formation:

\* the temperature, i.e., the activation energy, and

the reactions for chain formation of NO.

The final amount of NO produced actually depends on much more than the highest temperature reached during combustion. It is also a function of both the time it is exposed to these temperatures and of the oxygen concentration. Of time, since if the NO formation were as fast as the combustion reaction the NO would follow the equilibrium concentration corresponding to the highest temperature (the first reaction above is much slower than combustion reactions except at high temperatures). As it is, it lags and forms well into the post flame region.

Figures 1 through 3 taken from the literature illustrate these points. The longer the gases are exposed to high temperatures, the





higher the final NO concentration. Some implications of this behavior are as follows:

- \* Higher thermal NO, for coal versus oil or gas;
- Larger furnaces often imply larger residence time with resulting increased NO;
- Rapid quenching of gases in postflame region will reduce ND; and
- Higher temperatures for gas flames could result in higher nitrous oxide production.



Figure 2 Replacing combustion air with Ar/O<sup>e</sup> eliminates thermal NO (distillate oil); Pershing et al (1974).



Figure 3 Net concentrations of NO resulting from various time→ temperature profiles in the presence of 3% O<sub>e</sub>; MacKinnon and Ingraham (1972).

The graphs of Fig. 4, taken from Edwards (1974) qualitatively describe NO formation. Based on what we know about temperature and oxygen dependency we show Fig. 5 also from Edwards, and conclude that thermal NO is a strong function of temperature and combustion excess air.



Figure 4 Formation of NO as function of time or length of reactor; Edwards (1974).

2.2.2 FUEL-NO

Fuel-NO is derived from the oxidation of fuel fragments which contain nitrogen atoms. In the preflame-preheating zone, organic nitrogen compounds like NH<sub>2</sub> and HCN are formed which are oxidized very fast--on the same time scale as the combustion reactions:

Fuel-N --> HCN --> NH, --> NO --> Ne

Fuel nitrogen can react by either of

 $RN + D_{e} -- NO$  (fuel lean favored)  $RN + ND -- N_{e}$  (fuel rich favored)

The amount of Fuel-N converted to ND is known as the 'ND yield'. Therefore, the second reaction has a low ND yield. These reactions are neither very temperature dependent, as illustrated in Fig. 6, nor very excess air dependent, and so it is no surprise that the reactions leading to fuel-ND are similar to those leading to prompt-NO.



Figure 5 Relationship of flame temperature and equilibrium nitric oxide concentration; Edwards (1974).



Figure 6 Flame zone temperature has little effect on fuel-NO (residual oil in  $Ar/O_{B}$ ); Fershing et al (1974).

2.2.3 THE WHOLE PICTURE AND FURTHER CONSIDERATIONS

Fig. 7 taken from the literature gives a good summary of the pathways to NO<sub>4</sub> during fossil fuel combustion. Fig. 8 presents in clear terms the effect of temperature and excess air on fuel-NO. For coal the situation is even more extreme since the amount of fuel-bound nitrogen is even higher than for oils.



Figure 7 Mechanistic pathways of nitrogen oxides Formation in fossil fuel combustion; Farmayan et al (1985).



Figure 8 Air-ND and Fuel-NO: A--with preheat (277 C) and B--no preheat; Pershing et al (1974).

We have discussed the basic parameters leading to NO formation in combustion. But in a real furnace other parameters can be crucial:

- fuel type: next section;
- burner nozzle: swirl versus no swirl;
- turbulence;
- type of furnace:
  - wall-fired versus tangentially-fired, Wendt (1980) and Thompson and McElroy (1985);
- > plant size, Häsänen et al (1986): -confinement, residence time: Akiyama (1987); and
- daily operation.

#### 2.3 FUELS AND NO.

We saw earlier how emission limits vary between fuels and how a major contributor to NO<sub>2</sub> emission is nitrogen chemically bound to the fuel: C<sub>2</sub>H<sub>2</sub>N. In this section we look at NO<sub>2</sub> emissions and their relation to fuel-N for the main hydrocarbon fuels. These fuels are in heavy competition with each other and the pollution each generates is becoming one of the variables influencing their effective cost.

Since fuel-N is an important variable in ND, formation--an overriding one for coal--we now present some data on the nitrogen content of some fuels. We should mention in passing that "waste fuels" and biomass can contain much fuel-N.

Natural gas can contain nitrogen but it is unbound and usually in quantities less than 1.5% by volume; so compared to the  $N_4$  in air, it is a small contribution to total N. The same low fuel-N content is true of other "clean" fuels such as refinery gases and light oils. But heavy oils, crude and coals have a significant amount of fuel-N. For these fuels fuel-NO<sub>4</sub> dominates over thermal-NO<sub>4</sub>. So the large difference in NO<sub>4</sub> emissions between these can be traced to the difference in fuel-N. The following table gives typical values found in the literature for the weight percentage of fuel-bound nitrogen.

Coal	Dil No. 6 (residual)	Oil No. 2 (distillate)
1.17	0.3	(.05
(.5-1.7)	0.3	
(around 1.	}	

Natural gas can result in lower ND, emission than these fuels because:

- it contains no bound-N --> no fuel-ND; and
- it needs lower excess air for efficient combustion --> lower thermal-NO.

On the other hand, with the higher flame temperature usually associated with natural gas, a slight increase in  $NO_4$  could be expected. The same can be said for propane.

A survey of the literature has revealed the typical average emissions given below:

	NÜ, (ppm)			
	×0₂	⊎ %O₂	g/10∎ J	
coal	9.7	475	290	
No.6	5.3	269	151	
No.2	5.5	120	67	
Natural Gas	4.8	139	71	

	coal	oil	gas	wood
industrial	120	67	59	R. a.
utilities	101	52	18	6.5
domestic	16	17	t3	6.5

Häsänen et al (1985) in a study of Scandinavian plants compiled the results given in Fig. 9.



Figure 9 Emissions from an "average power plant" per unit of fuel energy; Häsänen et al (1986).

A recent survey by Vaclavinek (1988) revealed the following relative emissions, with natural gas being assigned a figure of 1:

Coal Heavy oil Light oil Nat. gas 2.3-1.8 1.4 1.1 1.

Natural gas produces lower overall NO<sub>x</sub> than the heavier oils of widespread industrial use. But for light oils, such oil no. 2, the emissions are comparable. These lower emissions of natural gas compared with other competitive fuels is reflected in the more stringent emission limits for gas! Dacey (1985) states that the general consensus for the emission limits are 50-60% that of coal for oil, and 30-50% that of coal for natural gas.

2.4 STRATEGIES FOR REDUCTION--NATURAL GAS CONTRIBUTION

#### 2.4.1 STRATEGIES

There are four general ways one can reduce nitrous oxide emissions from combustion plants:

1. Use the least pollutant fuel

\* Use natural gas!

2. Change operating conditions

\* Lower excess air

\* Load reduction

\* Lower preheat

#### 3. Combustion modifications

\* Low ND<sub>1</sub> burners

\* Two-stage combustion

\* Three-stage combustion (reburning)

\* Flue-gas recirculation

- \* Water injection
- \* Fast heat removal from flame
- 4. Post-combustion treatment

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\* Selective Catalytic (SCR):

The post-flame gases are passed by a reducing catalyst favoring reactions of the type:

 $2NO + 2CO \langle -- \rangle N_a + 2CO_a$  $2NO + 2H_a \langle -- \rangle N_a + 2H_aO$  $4NO + CH_a \langle -- \rangle 2N_a + CO_a + 2H_aO$ 

To reduce emissions, an obvious choice would be to switch to natural gas firing since we have shown that for industrial applications it is in most cases the least polluting fuel. Natural gas can also play a role in option two listed above. In general, following this course of reduction impacts adversely on furnace efficiency or capacity. But natural gas does work at lower excess air without a drop in efficiency versus other fuels. Even in cases where other fuels are of choice natural gas can still play a role in NO<sub>x</sub> reduction as we will see next.

Combustion modifications are perhaps the most cost-effective techniques for emission reduction, Maulbetsch et al (1986). The combustion modifications apply as well to natural gas as to other fuels: we can take advantage of low NO<sub>x</sub> burners and two-stage combustion as viable methods to reduce natural gas emissions. Furnace design and location of the flame with respect to furnace walls and load can be done as to increase the rate of heat removal from the flame thereby reducing its temperature. Sometimes this is easier to accomplish for a gaseous fuel than for a liquid fuel. As illustrated during a recent field trip to Svenskt Stål AB, one of the older preheating furnaces burning oil is operating as depicted in Fig. 10A below. The mixed droplets of fuel burn on the refractory



Figure 10 A-Oil flame; B-Expected gas flame. Observations from a trip by the author to Svenskt Stal AB, Borlänge, 1988.

walls and sometimes on the steel itself. With a planned switch to natural gas the situation as described in Fig. 10B is expected. The gas can follow the refractory roof resulting in good heat transfer to it and reduction of an otherwise quite hot flame temperature. This method of using a flat flame, see Chedaille and Koopmans (1973), (References 1) is one way of increasing convection from the gas flame and minimizing NO<sub>x</sub>.

#### 2.4.2 STAGED COMBUSTION AND REBURNING

Because of its importance this section will be separately devoted to combustion staging and to how natural gas is an ideal fuel for reburning. Staging, as the name implies, divides the combustion process into several reactive stages. Fig. 11 shows how this is accomplished. Staged air injection, also known as two-stage combustion, can be understood with the help of this figure. By having combustion occur away from the stoichiometric point all the fuel can still be burned while avoiding much of the NO<sub>2</sub> production. One way of doing this very compactly is by the use of a low NO<sub>2</sub> burner. Fig. 12 shows how this type of burner works. Glarborg et al (1987) and Collin and Vaclavinek (1984) present several types of low-NO<sub>2</sub> burners.



Figure 11 Principles of staged combustion; Hadvig (1987).



Figure 12 Low-NO, burner; Chugai Ro Co. Japan (1988).

For some fuels in which high amounts of NO<sub>4</sub> are generated (say an order of magnitude or more than natural gas) another type of staged combustion becomes advantageous: staged fuel injection, also known as reburning. This particular technique has been discovered over 30 years ago; it is based on NO destruction by hydrocarbons. This method is also important because it opens up the possibility of having low NO<sub>4</sub> operation while combustion proceeds at very high temperatures, such as those demanded by thermophotovoltaics, Felka et al (1987).

What makes reburning work, Fig. 13, is that fuel added into a reducing zone (low O concentration) consumes the already formed NO generated in the previous stage--NO becomes the fuel oxidant. In a fuel-rich zone the following NO reduction mechanisms can take place, Knill (1987),



Figure 13 Principles of reburning; Hadvig (1987), Heap and Folsom (1986).

Natural gas, and of course propane, are very good reburning fuels because, on the one hand they contain no new fuel-N to add to the final stage, and on the other hand, because mixing is very important during the final combustion stage gases are ideal. Fig. 14 taken from a recent International Flame Foundation Research report, Knill (1987), gives a good idea of natural gas performance in reburning.



Figure 14 Effectiveness of different fuels in reburning, Knill (1987).

#### 2.5 SUMMARY

- The environmental risks associated with nitrous oxides are covered together with representative governmental limits on their emission from fossil fuel combustion.
- NO<sub>x</sub> is found to be formed by two major pathways: thermal-NO and fuel-NO; the chemical/kinetics and the parameters influencing the formation paths are covered. These include temperature, excess air, air residence time.
- Measurements by workers taken from the literature compare ND, emissions for a variety of fuels. Natural gas is found to emit less than heavy oils and there is general agreement that it is the cleanest fuels in all studies.
- The major techniques for NO<sub>x</sub> reduction are presented. These include running at lower excess air, using low-NO<sub>x</sub> burners, and combustion staging. Attention is drawn to the fact that natural gas is a good reburning fuel since it mixes well and has no fuel-bound nitrogen.

CHAPTER 3: MATHEMATICAL MODELING: RADIATIVE HEAT TRANSFER

#### 3.1 GENERAL CONSIDERATIONS

To quantify the change in furnace performance when switching from oil to natural gas, a model must be able to predict the significant differences between the two fuels. This can be done in two different ways: by mathematical modeling, and by gathering experimental data from actual furnaces which have been modified (or by running controlled laboratory experiments with the various fuels). A literature search can also reveal much about this topic.

Sophisticated mathematical modeling can be used to predict performance but several problems arise with this approach:

- expensive/licensing;
- detailed information on burners, the fuel, etc, is required;
- the model might actually not account for some of the more important aspects of conversion; and

(The last point needs some elaboration. Many commercial codes which predict flow and combustion in detail often do not account for soot concentration in the flame nor for nongray gases.)

require expert knowledge to implement.

This modeling certainly has a place in detailed implementation by the furnace user of modifications, but a preliminary assessment of performance changes might be done more effectively with a simpler model. This we might call, for our purposes here, 'engineering modeling." Modeling, and in particular engineering modeling, of different fuels as far as impact on furnace performance has been done by many workers as mentioned in chapter 1: Wu (1969), Michelfelder and Lowes (1972), Abbott (1977), Hottel and Sarofim (1978), and others. Many of these approaches neglect the aerodynamic/reactive aspects in the furnace chamber and concentrate instead on radiative heat transfer given some assumptions about the fluid dynamics and the reaction progress. Sometimes convection is accounted for by assigning a mean convective heat transfer coefficient to the walls.

A complete comparison of oil and propane with natural gas would have to include the fluid dynamics of reactive flow and detailed information on burner geometry. This is outside the scope of this work and so this chapter will concentrate on the radiative heat transfer aspects. These are, of course, very important since the main mechanism of heat transfer in furnaces of industrial size is radiation. And so, comparing fuels can be reduced to comparing their radiative performance. For the most part this has been the approach taken by the workers mentioned above and it will be the one taken here.

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> In boilers convection is also very important and accounts often for over 50% of the total useful heat transfer. But this heat exchange occurs in the convective section of the boiler. We are here concerned with the radiative section--where the flame is and the combustion takes place--since we would like to determine wether the products of combustion of natural gas can be reasonably modeled with a simplified radiative analysis. Refer to Fig. 1.

> A discussion of radiative transfer for the various fuels leads one to the argument of accounting for spectral effects. This is because oil flames are more gray than natural gas flames and therefore, a correct prediction of performance changes when switching

itself with modeling the heat transfer of the products of combustion to determine when to use a simplified analysis. In the process, a literature search on this topic will be done.

## 3.2 RADIATION FROM COMBUSTION PRODUCTS: SPECTRAL VERSUS NONSPECTRAL CHARACTERISTICS

The medium in a furnace or boiler chamber is composed of a mixture of unburned hydrocarbons, combustion products, air, polydispersions, and pollutants. For radiative heat transfer we need concern ourselves with those components which emit, absorb, or scatter radiation and which are present in concentrations significant enough to do so. For gases, those components will be carbon dioxide and water vapor. The suspended solids will vary much in size, shape, constitution, and in radiative properties. Some simplifications can be made here for our purposes.

For the combustion of coal and other particulate fuels such as biomass, the scattering of radiation can be quite important and usually the particle size falls in a region in which scattering simply cannot be neglected and recourse to more sophisticated theory is necessary. Fortunately for us in this report the polydispersions are negligible in the case of gas (unless sooting is artificially induced) or the particulates are so fine as to make scattering negligible--the case with oil combustion. For our purposes we will call the fine mixture of unburned hydrocarbon chains and particles, and other tiny suspended particulates soot.

Soot radiation is qualitatively different from gaseous radiation but these differences we will leave for the following sections. In this section we will concentrate on the general treatment of a furnace chamber enclosing an emitting-absorbing medium which can be gray or spectral, i.e., emission and absorption are independent or dependent of wavelength, respectively. That dependence can be a

continuous function, as for the case of soot, or it can be discrete or banded, as for gases.

Fig. 2 depicts a general geometry for a furnace or a boiler. The difference rests essentially on the types of boundary conditions: the level and the relative temperatures of the walls. To simplify our terminology we will from now on refer to the two simply as furnace and bring back the term boiler when it is appropriate to do so. An evaluation of the heat-exchange in this enclosure involves two physical entities: the walls and the intervening gaseous medium. Each small surface element on the wall possesses a temperature, an absorptivity, and an emissivity (as well as a local convective heat transfer coefficient). Each volume element in the chamber will have a temperature, a concentration for each species, and an emissivity and absorptivity. The volume element can also have a certain chemical heat release from fuel combustion.

We will here treat the chemical heat release only implicitly: as it affects species concentration and temperature distribution. To organize the discussion we will now introduce some working definitions:

Diffuse surface: Radiative properties are not a function of incoming or outgoing angular directions. A standard assumption, one which we will follow, is that the furnace walls are diffuse.

Black surface: The theoretical maximum radiation is emitted and absorbed, and is only a function of temperature. The absorption and emission of radiation follow a planckian distribution as a function of wavelength, 1.

Gray surface: If the absorption and emission of radiation are not wavelength-dependent and emit less than the amount of a corresponding black body at a specified temperature, the walls are considered gray. We can also say that if at any wavelength

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the ratio of the energy emitted to that emitted by a black body is constant throughout the spectrum the surface is considered gray. If further the emissivities and absorptivities are not a function of temperature we will call these properties constant. A wall can also be emissive-gray,  $e\neq e$  (wavelength) yet be absorption-spectral,  $a\neq a$  (wavelength) and vice-versa.

Constant wall temperature: We will take each furnace face to be at a constant wall temperature. For a boiler all walls will generally be taken to be at the same temperature. For a steel or a glass-melting furnace, for example, one wall will be at the load temperature while others will be at an equilibrium refractory temperature.

Homogeneous medium: When the species concentrations and temperatures are invariant with spatial location in the furnace. Otherwise the medium is nonhomogeneous or inhomogeneous. Notice that we could have an approximately isothermal furnace chamber and yet still have a nonhomogeneous situation if, for example, the soot concentration is higher in one zone than in another. Homogeneity is related to the idealization of a well-stirred reactor: the mixture therein would be homogeneous in both temperature and concentration.

**Gray-gas:** A gas or mixture of gases whose absorption coefficient is not a function of wavelength of radiation. These properties, though, can be a function of temperature. Otherwise we will call the gas a real gas. Fig. 3 gives a conceptual clarification of these concepts.

Now we can take a realistic case for the furnace and list the combinations of thermo/radiative options for the homogeneity and for the radiative properties. We will have each wall be diffuse-gray. Then the mixture it encloses can be, in increasing order of complexity:

- 1. homogeneous-gray
- 2. homogeneous-nongray
- 3. nonhomogeneous-gray
- 4. nonhosogeneous-nongray

We can explain these four cases by taking the case of a pencil of radiation (emitted by a wall, say) and transversing an absorbingemitting medium. Refer to Fig. 4. These are directional properties and the intensity is likewise directional. Total energy transfer would require evaluation of the integration of the beam over all solid angles.

#### 3.2.1 HOMOGENEOUS-GRAY GAS

In this case the absorptance, a, of the gas is given by Bouger's Law, see for example Siegel and Howell (1984):

$$a = I(x)/I(0) = 1 - exp(-Kx)$$
 (1)

Where K, the absorption coefficient, is not a function of position or of wavelength.

Similarly, the energy emitted by the medium, the emittance, which is added in the direction of the pencil of radiation is given by:

$$e = I_{h}(x)/I_{h} = 1 - exp(-Kx)$$
 (2)

Where  $\mathbf{e}$  is the emittance and  $\mathbf{I}_{\mathbf{e}}$  is the planckian black body emissive power corresponding to the gas temperature. Notice that in general **a** will only equal  $\mathbf{e}$  when the source temperature and the gas temperature are the same.

This case then seems to offer no difficulty, and it is indeed the simplest situation one can find. But is it realistic? Are there any examples? For a medium with low spectral dependence, such as a This case then seems to offer no difficulty, and it is indeed the simplest situation one can find. But is it realistic? Are there any examples? For a medium with low spectral dependence, such as a heavily sooted flame or some zones of a fire with heavy smoke, the absorption and emission of the medium can indeed be approximated this way, Bard and Pagni (1981). Surprisingly perhaps, many sophisticated simulations of furnace radiation use this assumption so as to avoid further complications. See for example Selçuk (1985). Commercial codes also use this simplified treatment.

#### 3.2.2 HOMOGENEOUS-NONGRAY GAS; RADIATIVE PROPERTIES OF REAL GASES

It is here a good place to explain the differences between a gray gas and a real gas as we first stated them in the previous section. For a gray gas  $\tilde{K}$  is not a function of wavelength and therefore it stays constant throughout the spectrum. If we refer back to Fig. 3 we can see that the radiation absorbed is a constant function of the planck distribution. So at any temperature, given the corresponding absorption coefficient, we can determine the energy at any spectral location as well as the total energy by integration of Planck's distribution. The latter would simply be:

$$I(x) = \int_{0}^{\infty} a I_{1b} \delta I = a \int_{0}^{\infty} I_{1b} \delta I = I_{b} (0)$$
(3)

Since a is a constant. This is the as eqn. (1).

;.;;

But for a real gas eqn. (1) applies only, i.e., is exact, at a single wavelength

$$a_i = 1 - \exp(-K_i x)$$
 (4)

This is Bougers law in a more general form. The important thing to realize is that the quality of radiation as it travels through the medium changes. Hypothetically, some wavelengths will be absorbed planckian distribution is entirely altered, and the spectral emission and absorption of energy can be quite a complicated function.

Further, a change in the source temperature will result in a change in a due to the spectral distribution of the source shifting, meaning it will go into a different zone of influence. This is shown schematically in Fig. 5.

Fig. 6 illustrates how the total emittance (integrated over all spectrum) if a gas is real, in this case water vapor, does not obey the simple exponential relations given previously.

But in a situation in which the medium is approximately homogeneous, we could take a 1-zone of dimension L, where L is a characteristic dimension or the length of the radiative beam, and we could calculate the amount arriving at the end quite accurately. So this case we could handle by using a curve-fit of the gas or mixture of gases and soot emissivity to define a suitable mean emissivity for the mixture as a function of L. These fits exist in various forms calculated by several workers:

1. mixture of gray-gases, Hottel and Sarofim (1967);

- 2. variations of 1.;
- 3. gases and soot, Taylor and Foster (1974);
- 4. curve-fits of gases and soot, Modak (1978).

These curve-fits are taken of experimental data. The oldest, and used most extensively by the practicing engineer and the scientist alike, are those of Hottel and Sarofim (1967). More recently new data taken by General Dynamics (1968) has been made available and correlated by Leckner (1972a). It is important to realize that these data are not written on stone. See for example Docherty (1982) for a discussion of their validity.

All methods have been used successfully but we feel Modak's method is most recent, quite accurate (with respect to experimental data) and includes soot contribution while spanning, a wide range of temperatures and species concentrations. It is the method we use in this report. The subroutine ABSORB as published by Modak in the above reference is used in our computer model.

How do these mean radiative properties work? By weighing the emissivity at a each wavelength with its respective black body intensity. For the total absorptance,

$$a(x) = \frac{\int_{0}^{\infty} I_{1}(0) (1 - exp(-a_{1}x)) \delta 1}{\int_{0}^{\infty} I_{1}(0) \delta 1}$$
(5)

Similarly for the total emittance,

$$e(x) = \frac{\int_{a}^{\infty} I_{k} b(T) \left(1 - exp(-a_{k}x)\right) \delta 1}{I_{k}(T)}$$
(6)

Notice how the detailed information about the spectrum is lost in the integration. Therefore we can only obtain total energy transfers, which is all we are after in many industrial cases.

We can illustrate this loss of information with an example. Say we have a curve-fit of emissivity, and let us take the case of a pencil of radiation crossing an emitting-absorbing, non-gray medium. The total absorption by the medium for a thickness L is given by:

$$a(L) = I(L)/I(0)$$
 (7)

And let us say that we wanted to know how much energy is being absorbed by the medium in a particular location of length dx. This would be given by the local absorptance:

#### a::+:+=: = I(1+1)/I(1)

For a gray gas

$$a_{11+11-1} = 1 = e_{X}p(-Kd_X)$$
 (9)

and since K is constant

$$a(L) = 1 - e$$
 (10)

But for a real gas the first equation does not equal to the second and instead:

$$a(x) = a(1+1)/a(1)$$
 (11)

The practical conclusion is that if we are interested in local energy transfer within a zone, the local dimension is not enough to specify it. Instead it is only computable as a function of the initial starting location: the history of the beam is required. For a gray gas we need not know the temperature and "history" of the beam of radiation whereas now we do.

We have seen in this section how a spectral medium can be treated by a proper use of total absorption/emittance properties. The medium of interest in our case would be products of combustion of natural gas.

#### 3.2.3 NONHOMOGENEOUS, GRAY GAS

Here the nonhomogeneities can be in the temperature field, or in the constituents' concentration, or in both simultaneously. The result is that if K is a function of temperature and/or of species, which it usually is, the absorption/emission will be varying in

(8)
space, in our case in the x-direction of the beam travel. Mathematically:

and

$$a(L) = 1 - exp(-\int_{0}^{L} K(x) \delta x)$$
 (12)

Notice if K = const, this equation simplifies to eqn. (1). If we know the temperature field, as a function of position, x, then we could conceivably find K by integration.

Let us again look at the practical case of dividing our medium into homogeneous zones. The intensity of the original beam of radiation at any point will be given by,

$$I(x) = I(0) \exp(-\int_{0}^{H} K(x) \delta x)$$
(13)

If we assume then that we can divide the path into n homogeneous zones, we can discretize the integral part of this equation:

$$I(x) = I(0) \exp(-K_1 dx_1 - K_2 dx_2 - ...)$$
 (14)

Since the medium is gray the absorption/emission in each zone is a local property, a function of the local geometry, dx, concentration, and temperature, so we notice no difference between this and the previous equation for a nongray gas,

$$I(x_{i+1}) = I(x_i) (1 - exp(-Kdx))$$
 (15)

and

$$I(x) = I(0) \exp(-K_1 dx_1) \exp(-K_2 dx_2) \dots$$
 (16)

but in general

$$a = 1 - exp(-Kdx)$$
 (17)

And we obtain

$$I(x)/I(0) \simeq a(x) \simeq (1-a_1) (1-a_2) \dots (18)$$

This case can also be treated rather simply given that every zone can indeed be treated as gray and that we can approximate the continuum into a series of finite zones. This analysis permits us to treat, for example, a combustion zone heavily sooted but with regions of varying temperatures and concentrations. Or a situation which is sooted-gray and another with only gases which we could neglect (a=0).

#### 3.2.4 NONHOMOGENEOUS, NONGRAY GAS

In this section we present the most general situation in which the medium has a definite spectral, usually complex, distribution and possesses nonhomogeneities in either temperature or species concentration in the enclosure under consideration. For the sake of completion we present the energy equation for our, by now familiar, beam of radiation. The radiative intensity at any point would be given in this most general case (recall we are neglecting scattering) by a double integral involving the space variable, x, and the wavelength variable, 1, see for example, Buckius and Tien (1977).

Since we have seen that radiation behaves quite irregularly throughout the spectrum, an exact solution is impossible. Solutions involve a discretization of both the spectrum and the medium. The finer the discretization the more exact the solution could become. Gases absorb in discrete steps throughout the wave spectrum, caused by absorption or emission of photons. These steps are seen as lines. Data are available for these narrow-bands, see Edwards (1976), but this method presents three basic difficulties:

- The availability of complete and accurate data for gases over the whole spectrum of interest;
- The amount of computer time required for even simple calculations is enormous at today's computing speeds; and

This scenario caused researchers to seek simpler discretizations of the spectrum. In thermal processes of interest to us these absorption lines are "blurred" by a process known as collision broadening. Gaseous absorption clusters around definite wavenumbers forming bands which can be characterized by a certain distribution. This resulted in the development of wide-band models, see for example Edwards and Balakrishan (1973). The spectrum is then discretized into bands centered around each wavenumber and the suitable mean absorptance for each band is determined. The result is that for each beam we trace in space the energy in each band is individually tracked. The total energy transmitted is the sum over n bands.

This method gives excellent results compared to the more exact spectral line method. Generally when researchers refer to spectral radiative analysis this is the method they are referring to. The wide-band model is actually used as the numerical yardstick to assess total absorption curve-fits and other approximate procedures. For example, Modak (1978) used it to do just this.

We know the engineer is by nature an impatient species with tight schedules and often without a fast computer at his or her disposal. Often the exponential wide-band model falls short of convenient implementation and speed of computation. Often the engineer will trade accuracy for expediency. To this end the methods of section 3.2.2 were developed.

Now we start with a question: In this situation can we approximate a real gas as an equivalent gray gas? Specifically to us in this report: can we model the radiative transfer from the products of combustion of natural gas in a nonhomogeneous field with good results? The answer is a qualified "yes!" since information will be lost from one homogeneous zone to the next as discussed in previous sections. Here is a situation in which one would be tempted to simplify this case to a method of the previous section. Let us take a nonhomogeneous furnace and track a beam of radiation transversing it. One would be tempted, when tracing the intensity of the radiation beams, to use a gray gas approximation for each control volume the beam crosses. We have shown in section 3.2.2 that this can lead to significant errors especially the higher the spectral character of the gas (true for most of furnace volume).

But are there approaches one can take short of full tracing of energy in each small wave interval? Indeed there are and these we will discuss next. Going back to the nonhomogeneous furnace, just mentioned, one simple approach worth considering is arriving at an equivalent homogeneous mixture, for the temperature say, and then applying the gray gas approximation to the whole of the volume. Since we have shown before how this can be modeled with good results we can approach this nonhomogeneous situation by developing suitable equivalent parameters. of concentration, temperature, and/or characteristic length.

Hottel and Cohen (1958) use a simple averaging for the absorption coefficient of the form:



when K is a function of species concentration which is varying in space. When the temperature of the medium is varying they make simple approximations on K based on the fact that first, often it doesn't vary by more than a few percent over a large temperature span and second, most emission/absorption will come from the furnace walls.

Leckner (1972c) defined the total absorptivity for a nonhomogeneous, nongray by calculating an effective "mean value of temperature" weighted by a partial pressure:

$$\overline{T}_{bAB} \stackrel{L}{=} \frac{\int_{-L}^{L} T_{bAB}(x) p(x) \delta x}{\int_{-}^{L} p(x) \delta x}$$
(20)

and on average partial pressure for the nonhomogeneous path.

Strömberg (1977) calculates a "radiative mean temperature" by weighing the gas temperature raised to the fourth power with the derivative of the local emissivity with respect to the spatial coordinate. He then calculates effective emissivity analytically for a furnace temperature with an elliptical temperature distribution.

Grosshandler (1980) is of the opinion that "neither narrow-band nor wide-band models are necessary to accurately model" nonhomogeneous mixtures of nongray gases. He presents a simplified model which gives results within 10% accuracy, runs quite fast and was verified for the parameter range of interest in furnace cases. The model is developed from the approximation of Leckner presented above. The reader is referred to Grosshandler's paper for full details. There are also other workers which the author believes have useful publications in the area of nonhomogeneous, nongray mediums of interest to furnace modeling: Krakow et al (1966), Edwards et al (1967), Plass (1967), Cess and Wang (1970), Edwards and Balakrishnan (1972), Buckius and Tien (1977), Grosshandler and Modak (1981), Tien and Lee (1982), and Docherty and Fairweather (1988).

Each of these approximations can be useful in modeling the spectral radiation of the products combustion of natural gas. If actual running codes are available is a different matter. It would also be very useful and perhaps a project to be taken up by the author, is an actual comparison of these methods in as far as accuracy and speed and ease of implementation.

But a simple approximation taken routinely by researchers is to merely average the furnace temperature and concentration in some simple algebraic manner. This is not so unrealistic, for example, Mengüç (1985) predicts that a variation of 100 K has little impact on radiative properties, especially if we consider all the other variables' approximations. The averaged properties of the mixture can then be attacked by the one-zone method of Hottel and using the analysis of section 3.2.2.

This can work well if the nonhomogeneities are not very high and an appropriate averaging procedure is done. Gibb (1987) shows the insensitivities of furnace modeling to the radiative parameter impact because of the typically large furnace dimensions. An extension of this approximate method known as the long furnace model has been applied with good results to furnaces possessing one-dimensional preference. The reader is referred to the works of Lowes and Heap (1971), Beér (1972), Lowes et al (1973), Ström (1980), Tucker (1988), Vaclavinek et al (1983). By dividing the furnace longitudinally into sections and treating each individually by the methods described in the above paragraphs, a reasonable treatment is accomplished.

Assumptions will of course be made on the transmission of radiation from one zone to the next and on the average temperature in each.

## 3.3 SOOT AND RADIATION INCLUDING SOOT

The presence of soot during the combustion of liquid (and solid) fuels results in a modification of the radiative environment within a furnace chamber vis-a-vis that of natural gas. Soot formation is a sign of unmixed, unburned hydrocarbons, and therefore most likely a sign of inefficient combustion! Despite its undesirability, a small amount of soot will always form during oil combustion which gives the flame its characteristic luminous yellow color.

If hydrocarbon combustion proceeds to completion the combustion products of interest to radiative heat transfer will be the same for oil and natural gas, namely, water vapor and carbon dioxide. But the proportions of the two will vary amongst oils and especially between oils and natural gas. Typically, the latter will result in partial pressures of  $H_{e}O$  twice as high as that of  $CO_{e}$ . For oils they are approximately the same. This partial pressure difference itself will result in different radiative characteristics as is well known, see for example Wu (1969).

Soot is a strong emitter of radiation so its impact will be more pronounced in smaller furnaces possessing a small characteristic length, i.e., smaller mean beam length. To quantify soot's impact on furnace heat transfer we need to establish the parameters affecting its radiative behavior.

It is then appropriate now to define what we mean by soot. As pointed out by Haynes and Wagner (1981), soot formed during combustion "is not uniquely defined." But we can arrive at a working definition:

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Soot is a mixture of carbon particles and conglomerates formed during the combustion of hydrocarbon fuels which is

fine enough to be treated as radiatively non-scattering.

Soot is usually formed under concentrations so small as to not require a reduction of the fuel enthalpy in the overall energy balance. But despite its small concentrations soot can be a strong emitter of radiation, especially in the visible portion of the spectrum, therefore flames containing soot are called luminous.

How is solt concentration given? Usually the choice is given in terms of what optical/radiative model the researcher is using. The most common is know as soot volume fraction,

f. = volume of sout / unit volume, m³/m³

Another definition is soot mass density,

f<sub>n</sub> = mass of sout / unit volume, g/m<sup>2</sup>

To connect the above quantities the mean specific soot density,

 $S_{d}$  = mass of soot / unit volume of soot, g/m<sup>3</sup>

needs to be known. The relation between the three quantities is given simply by

 $f_{\Psi} = C * f_{\Psi} / S_{A}$ 

where C will be a constant to accommodate the particular set of units we might use. The only reference the author has found on such a specific soot density is that given in Taylor and Foster (1974), which gives

 $S_d = 1.65 \ 10^3 \ Kg/w^3$ 

This value can of course be debated but one can take some consolation in the fact that using it there is a consistency of resulting values. Soot density is known, for example Zethræus (1988), to fall somewhere between 0.3 and 2 gram in the flame zone, sometimes extending to 5 g, in an heavily sooted flame. Using these figures we could get

$$f_{\bullet} = 1.8 \ 10^{-7} - 1.8 \ 10^{-6}, \ m^2/m^2$$

This value falls in the range given in most studies for soot concentration, 10<sup>-\*</sup> to 10<sup>-\*</sup>. Of course, this is a span of two orders of magnitude, so we need to be more exact than this for an actual furnace calculation.

Though much is written about soot and about the fact it is produced and "seen" in oil flames little can be found that can answer the following:

"I have a furnace with so and so characteristics, running at so much excess air with this fuel; what is the soot concentration in the flame itself and in the remainder of the furnace chamber?"

Many measurements are carried out for a single flame, group of flames, and fires, under laboratory conditions, for example Beér and Claus (1962), Gaydon and Wolfhard (1979), Bard and Pagni (1981), Kent et al (1981), Prado et al (1981), Grosshandler and Vantelon (1985), and Habib and Vervisch (1988). These works offer us an in depth understanding of soot forming mechanisms, but fall short of answering the question we placed above. A more industrially useful work was presented by Hein (1970) of the International Flame Research Foundation, by Peterson (1972), Peterson and Skoog (1973), and Peterson (1981).

Generation of soots from fuel oils depends on such factors as:

- Oil type;
- Excess air;
- Load; and
- Burner type.

Dil type appears to be the most important parameter affecting soot formation. Unfortunately, soot formation does not correlate well with the Standard classification for oils which is essentially a rating of viscosities. Therefore a fuel oil number 5 does not necessarily emit more soot then a fuel oil number 3. Indeed, Peterson and Skoog (1973) have shown in measurements of oils all falling within Class EO 4 that emission of soot and "dust", can vary by a factor of 30.

Peterson (1972, 1981) has shown that soot is correlated better by the amount of very heavy molecules, asphaltenes, contained in the oil. During combustion these molecules give rise to cenospheres which emit visible radiation and which might not burn completely before exhaust to the atmosphere.

The conclusion is that we cannot predict beforehand what the soot emission form an oil furnace will be wintout having made measurements on the particular oil it is using, etc. This does not present such a big problem for the users of this report and of the model provided with it—the model aims at predicting furnace performance with natural gas—performance with oil is already available for that particular furnace.

To predict oil emission we need to supply the model with an estimate of soot concentration or perhaps the best we can do is to supply a reasonable range of values and the author feels this is the best we can obtain from the literature at this point.

Now that we have discussed soot concentrations in a flame and in the furnace chamber we need to determine the impact of soot

concentration on radiative heat transfer. There are several works detailing the optical properties of soot. These properties are a function of the fuel burned, the number and shape of the particles and their conglomeration, density, the flow field. Along these lines we have the work of Bard and Pagni (1981), Habib and Vervisch (1987), Charalampopoulos and Chang (1988), and others.

It is generally agreed, for example Mengug and Viskanta (1985), that since the mean soot particle size is small scattering is negligible. The Wie theory of particle scattering states that it depends on the parameter (mD/l)\*. Where D is the particle diameter and 1 is the wavelength of radiation. Since in furnaces the temperature leans to the infrared, and the sout particles have quite a small diameter this value is much smaller than the absorption coefficient proportional to (mD/l). Scattering can then be neglected. The result is obtained in the small particle limit of the Mie equations that the soot absorption coefficient is not of function of particle size and size and distribution, Sarofim and Hottel (1987). shown theoretically and has been shown Further, it can be experimentally that the spectral soot absorption coefficient is continuous and inversely proportional to wavelength:

# K<sub>1</sub> = #(1/1)

Therefore we can expect soot to emit (and absorb) more at higher temperatures, since the blackbody spectrum will be shifted to shorter wavelengths. Fig. 7 from Habib and Vervisch (1988) presents what we can take as a typical absorption coefficient distribution for soot. This figure also points out the importance of soot in flame radiation itself.

One tends to take sout has being gray because of the fact it absorbs continuously, and because, since the emissive power at any particular wavelength is given by the product **e**,**E**,**b**, when we consider

 $E_{10}$  is also varying, we have an only sightly varying soot emissivity, Yuen (1976).

The relation between K and concentration is found from several sources, for example, Taylor and Foster (1974) give

 $K = f(f_H), g/a^3$ 

Modak (1979), which we will use, gives

by the relation

 $K_0 = 7 f_{\rm F}/l_{0}, 1/{\rm H}$ 

Where  $l_0 = 0.94 \ 10^{-4}$  m.

Having established the radiative properties of soot we need to combine them with those of the real gases,  $H_{e}O$  and  $CO_{e}$ , to evaluate their combined effect on furnace heat transfer. Since soot is assumed to not scatter, its radiative characteristics can be incorporated directly into correlations for the gases.

Accounting for a mixture of soot and spectral gases considering that their absorption curves overlap means we cannot simply add the emissivities of gases to that of soot. The total emissivity can be given by:

# RHINT T REDUT + REABES - REVERLAP

This relation is instructive because it gives a physically clear picture of the situation. For low soot concentrations the second term dominates. The gaps between the gaseous absorption bands are bridged by the soot emission and the mixture becomes less wavelength dependent: more gray. Fig. 10 taken from Docherty and Fairweather (1988) reproduces well this phenomena.

So, for an oil-sooted flame, we could neglect the spectral gases but for the bulk of the furnace but since it usually does not fill the whole chamber then the spectral/gas radiation has to be included in some form. The important thing is that in general if we have a correlation for a mixture of real gases and soot it should be used. Luckily those correlations exist and the fact they were developed means that there are indeed a large range of applications for which they are suitable and give good results.

We have mentioned the works of Taylor and Foster (1974) and Modak (1979), amongst others. These correlations are very practical because they include the mixture of the two gases and soot and reproduce the data of Hottel quite well for large concentration and temperature ranges but it is important to keep in mind that they apply under the conditions of homogeneity and for total heat exchange between one gas zone volume and its surrounding walls. When we need to divide the furnace into zones and apply such methods as discrete transfer method (1981), these curves have to be used with caution. This we discussed before in section 3.2.2.

Flame emissivity is clearly higher for a luminous flame than for its nonluminous counterpart. But the matter does not end here. The flame does not fill the whole combustion chamber, and often fills only a small portion of it. Further the strong absorption of the flame can actually block the load from wall radiation. This phenomena as been well documented in the literature. We can consult many references detailing this: Lee et al (1984), Viskanta and Mengüç (1987), by Docherty and Fairweather (1988). Fig. 8 clearly shows this soot blockage effect. And, of course, luminosity is often a result of bad combustion, resulting from bad fuel/oxidant mixing, fuel droplets, etc.

One concern in modeling the different radiative behavior of the two fuels, is the spectral characteristics of their products of combustion, as we have already seen. For natural gas these are strongly banded-spectral, and for oil these are continuous-spectral due to the smoothing effect of the soot concentration. In practice these differences are reduced by the fact that, first, absorption and re-emission by the walls increases the "grayness" of the chamber and smooths the spectrum; second, in many situations an approximate accounting of spectral behavior by deriving a globally equivalent gray gas results in quite accurate solutions of practical problems. (especially true for quasi-homogeneous mediums.) When more than integrated quantities, such as overall heat flux and average wall temperatures, are required, or when the furnace chamber temperatures and species concentrations are highly nonhomogeneous, a spectral treatment of radiation is required, as covered in section 3.2.4.

The ratios of water vapor to carbon dioxide are quite different for the two cases. Typically, they are one-to-one for natural gas and one-to-two for oil. Since water vapor is a better emitter than carbon dioxide, a natural gas-fired furnace will deliver more radiation to the load than an oil-fired furnace with no soot. Fig. 9 shows this effect.

Ideally, the complete combustion of heavy oil should be accomplished with, say, 5% excess air. In practice, it is common to run an oil furnace at 10% excess air and sometimes at 20%, whereas for natural gas, with mixing and combustion occurring smoothly, 5% excess air and less is typical. The result of running at higher excess air is that the energy of the fuel is increasingly used to heat up unnecessary molecular nitrogen and oxygen in the combustion air. This results in a lower furnace temperature and in increased stack losses. Davies and Deppen (1972), documented this quite well when they compare the heat transfer from oil and gas at various air flows, Fig. 10.

The fact that heat transfer for natural gas relies less on flame heat transfer and that the gases are more radiative due to higher water vapor content means that heat flux within the furnace is more evenly distributed throughout the furnace than for oil combustion. Wu (1969) has shown this effect for the case of a long furnace.

## 3.4 SUMMARY

- After listing some of the difficulties in running complex models the case is made to develop a simple furnace radiative heat transfer model. This model must be capable of accounting for the spectral radiative characteristics of natural gas combustion products.
- To proceed we looked at the various situations one could encounter in a general enclosure containing a homogeneous or nonhomogeneous, gray or nongray medium. The four combinations are covered by simply studying one beam of radiation transversing the medium. In the process a clear understanding of spectral versus gray radiation arises.
- The real gas (nongray) versus the gray gas are discussed and their characteristics compared. It is shown that total energy flows across one homogeneous zone--homogeneous, nongray--can be computed accurately and several curve-fits of gas/soot mixtures<sup>1</sup> radiative properties are available in the literature.
- The more general and complicated case of nonhomogeneous, nongray medium, is covered and approximations from the literature are presented to show how this system can be simplified in many cases to the previous one. For a global, simplified model of a furnace this case can be then treated in an approximated yet accurate manner also.

Formation and radiative properties of soot are treated. It is shown how soot influences medium radiative behavior. Soot can be incorporated relatively simply into emissivity curve-fits, since it is essentially non-scattering, for total gases' properties. It is concluded that the presence of soot in a furnace does not necessarily increase its efficiency. Soot blockage of the walls has been well documented.



Figure 1 Radiative section and convective section of a boiler.





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Figure 8 Soot blockage; Docherty and Fairweather (1988).









### CHAPTER 4: MODEL DEVELOPMENT

## 4.1 GOALS

In Chapter 3 we covered the principles behind radiative heat transfer; we considered a particular line of sight or "pencil of radiation" crossing an emitting-absorbing medium. To apply those concepts to actual furnace modeling we need to go further and consider the geometry of the system with the result that we will have not one beam of radiation but and infinite amount.

Our goal for this chapter is to take this complex problem which when analysed differently results in difficult nonlinear differential equations, Viskanta and Mengüç (1987), requiring numerical methods for their solution, and are only analytically solvable in the simplest of cases, and develop a simplified global model satisfying the following criteria:

- Applicable to a large range of box-type geometry furnaces and boilers;
- incorporate nongray approximations of gas/soot mixtures' radiative properties;
- predict the differences in capacity (exit temperature and load) and efficiency between an oil-fired and a matural gasfired furnace;
- allow for individually specified walls;
- to run on a personal computer in the order of a few minutes;
- to be user-friendly.

It is also important to state what we are not expecting the model to do:

- To give heat flux or temperature distributions for the walls;
- to predict or use medium temperature and species' concentration distributions---instead, the properites will be averaged into a well-mixed homogeneous mixture;
- to be a design tool for new furnaces, except at an early stage of development.

The main purpose of the model is to compare the relative differences in operation caused by fuel changes in furnaces and boilers, specifically, for different fuel-oils, natural gas and propane.

Any worker in the field knows that actually no furnace is a cylinder, or a paralelipied, or infinitely wide, or two-dimensional, but he or she also knows that very good practical and accurate results can be obtained with these simplifications. With this in mind we can refer to Fig. 2 of chapter 3, and claim that this generic geometry is indeed typical of a large assortment of furnaces, boilers, and industrial ovens, by merely stretching or contracting one of its dimensions. For example, stretching the furnace along the horizontal direction we would have a "long furnace" typical of heat treatment processes, conveyorized processes, etc. Flattening the height we could have a glass melting pool, for example. Make the three dimensions about the same and we could have the radiative section of a boiler or of a district heating plant. An added complexity which we will not take up here is that these changes in geometry are also accompanied by changes in the amount, type, and location of the burners. Since we are developing a well-mixed combustion chamber this will not be accounted for.

We can classify the furnace as according to its: 1. geometry; 2. boundary conditions; and 3. state of homogeneity in the chamber. The boundary conditions refer to the six walls:

- are they black or gray?
- are all at the same temperature?
- have the same emissivity (for non-black)?
- can we give each wall a realistic constant temperature?
- is there other heat transfer modes besides radiation? (e.g., convection from hot gases or conduction (heat loss) to the outside environment)

The geometry has implications for the walls and for the homogeneous assumptions. For example, it is rather obvious that a "long furnace" will result in flow downstream being different than flow upstream, so that wall temperatures will vary from up to down stream, and so will the chamber mixture's, temperature and concentrations. Therefore we could state that deviations form cubic geometry will call for a more detailed treatment of the furnace: its divisions into "zones" or into spatial grids of properties.

The type of burner, the amount of swirl, flow rates with respect will to furnace valume also either increase or decrease nonhomogeneities. As an example of relatively well-mixed flow, a tangentially-fired boiler in which recirculation is strong, turbulence and swirl are high and we would expect extensive mixing. On the other hand, furnaces in which the flames will occupy a small space will have large concentration and temperature gradients.

In other words, a relatively large group of cases could be studied each with a prominent feature. And this has indeed been done by a large number of researchers and engineers over the years. Many variations of models have been presented and the reader is referred to the following references which have special relevance to our topic: Beér (1972), Emmerich et al (1988), Lowes and Heap (1971), Lwes et al (1973), Michelferder and Lowes (1973), Scholand (1978), Song and Viskanta (1988), Ströw (1980), Tucker (1988), and Wu (1969).

We will now curtail the discussion here since we would be deviationg from our simple model. But one important point must be made. Often one will find in the literature sophisticated discretization of radiation problems, for example, Selcuk, Menguc, Kent, yet discover that the absorption coefficient for the gas mixture will be taken to be constant. These, we must stress, are not minor simplifications. For example, making walls nonblack forces a simple application of the Discrete Transfer method, Lockwood and Shah (1981), to become an iterative solution. Nonconstant K throws us into the foes of nongray-nonhomogeneous mediums as discussed in the last chapter. Seen in this light, a simple model with physically realistic assumptions can lead to very useful results. To that end we now devote the remainder of the chapter.

#### 4.2 MODEL DEVELOPMENT

Development of a simplified model consists of four sections:

- Assumptions: does the model proposed illustrate the differences betweeen oil and natural gas, i.e., does it account for differences in gray versus nongray radiation?
- 2. Propose and develop model.
- 3. Numerical implementation.
- Validation and application (some cases studied by our model and how the results compare with the literature).

Siven the time schedule of the project, abiding the desire to

have a fast runing model, and confident that good results can be obtained by a simple model, the proposed model is characterized by:

Geometry: Box-type.

Walls: Nonblack, diffuse, individually specified emissivities and temperatures or heat flows; radiative equilibrium (conduction and convection heat transfer are zero).

Medium: one-zone, well-stirred homogeneous combustion and mixture of combustion products and soot; given this, the analyses for homogeneous-nongray medium applies.

Since each wall as a whole can have its own thermal characteristics we have to treat its radiative interchange with each other wall and with the mixture as a whole. The analyses here follows the standard procedure, see Siegel and Howell (1981), of the net-radiation method. In this procedure an energy balance is applied to a three dimensional enclosure with n-surfaces enclosing an emitting-absorbing medium.

This formulation is quite general and can be integrated over wavelength. In practice to tackle it we could divide the spectrum into bands over which certain properties could be taken as constant, this would lead to a "wide-band model", Edwards (1976a). Or we could take an average over whole the spectrum, and arrive at overall transmittance, emittance properties. The latter is the procedure followed in our current model.

We are left now with determining these values. Again we could use several methods. We will use a method published by Dunkle (1964), and used with very good results, Siegel and Howel (1981). We will not detail here Dunkle's treatment or assumptions, that is done well by the author and discussed by Edwards in the original paper. The major approximation lies in assuming a linear absorption law for the gas. By approximating the absorption by a linear function we are left with a geometrically dependent integral which can be tabulated for various geometries. For our enclosure, these are the perpendicular rectangles sharing one side, and the directly parallel rectangles. Explicit equations are given for these by Dunkle and are used in our model. This characteristic length is used to obtain the emittance between each pair of surfaces.

In general the gas will be at a temperature different than the wall. So emission will not equal absorption. To account for this the original work by Hottel (later refined by Edwards (1976b)) is used. We are now in possession of a square matrix of sixth order, i.e., with six unknowns. The unknowns can be any combination of wall heat fluxes or wall temperatures. We still don't know the gas temperature. Of course, we could simply specify it but in a realistic situation we would not know this value à priori. The approach we take is to provide a certain fuel flow rate at a certain level of excess air. Then energy conservation with no combustion air preheat will give:

Energy released by fuel = useful energy removed by wall(s) + energy carried by exhaust gases

Where we assume T  $_{RIXTURE} = T_{SXNAURT}$ , to be consistent with our assumption of a well-stirred reactor.

The model could be optimized in the future for faster computation. The convergence procedure is slow but certain--given physically realistic imputs as discussed in the Manual. It could also, of course be modified to fit the users needs, include preheat, and to improve its approximations as well.

#### 4.3 MODEL VALIDATION

In validating the model we should aim to check expecially certain aspects. Namely,

- To what extent can this "box-type" model be used for "long" furnaces?
- To what level of accuracy does it predict the performance fo gas-fired furnaces versus oil-fired furnaces?
- Whether it predicts trends correctly.
- To stipulate the bounds (limits) on its operating range, outside which its results will be misleading.
- Whether even for the expanded operating range it indeed gives accurate and useful results.

We will make here a first attempt at this complete validation by running some checks:

- Self-consistency;
- A FLUENT run; and a case in the literature.

Consistency does not in itself validate the model but it is the first step to be taken to detect gross errors. We aim to determine whether the model "makes sense". To do this we run several simple cases for which we can use intuitive reasoning coupled with physical laws as checks. In other words, does the physics of the answer given by the model make sense?

We can look for the following indicators of trouble:

Energy balance;

- Symmetry;
- Violation of physical laws, e.g., second law; and
- Right order of magnitude.

Several simple cases were run, which of course the user can easily duplicate, to insure all these criteria were met. These simple checks showed that the model is indeed making "physical sense."

We also had at our disposal predictions for a real boiler obtained with a commercial, FLUENT, to see actual performance comparisons. These results were presented recently by Collin and dos Santos (1988). The boiler characteristics are as follows:

dimension: 6 \* 6 \* 6 m emissivity of walls: 0.95 (?) fuel flow rate: 57 MW oil No.4 temperature of walls: 250°C excess air: 15% soot concentration: 0.0 (?)

Some input values to our model are uncertain (?) since we were not positive on the values used by FLUENT. The predictions for the radiative section of the boiler are as given in Table 1.

TABLE 2				
<u></u>	FLUENT	THIS MODEL	. % DIF	****
RADIATIVE OUTPUT	23.91 MW	21 MW	12%	
EXHAUST TEMPERATURE FROM RADIA-	10 <b>50°C</b>	1266°C	-19%	
TIVE SECT. O:58 RUN TIME (min:sec)	Compa <b>d</b> 386 NA	39 2:40	Bondwell	286

Validation model takes running many cases, some of a experimental, and fine-tuning to increase prediction accuracy. One case form the literature is now compared. It involves a very longfurnace presented in Scholand (1978). For this case of strong deviation form a "box" geometry we would expect the model to be less accurate than for the previous case of the boiler. Further, this particular furnace is cylindrical and we approximate it with our cartesian coordianates as a long box. The length is 5 meters and the diameter measures 0.9 meters. The experimental results give, refer to paper, total heat absorbed by load of 0.5 NW, whereas the model overpredicts by giving 0.5 MW. Some of the discrepancy is due to the fact we don't have all the operating conditions at our disposal.

4.4 ILLUSTRATIVE USES OF THE MODEL

In this section we apply the model just developed to some situations which could arise in industry and which throw some light on the radiative differences between oil-firing and natural gas-firing. These will address soot concentration, and the  $CO_{4}$  and  $H_{4}O$  partial pressures differences between fuels.

Even though the model works for oils as well as for natural gas, that is, for furnaces with visible flames as well as for furnaces with blue flames, care has to be taken with the oil cases. The assumption of well-mixed furnace chamber containing only products of combustion is merely a rough approximation. The performance is quite sensitive to soot concentration and these values will be hard to determine and input. We could say, as we discussed in section 3.3 that the model would simulate better natural gas than oils because of the sooted flame.

The best use of the model is that which would actually occur in practice with potential Swedegas costumers:

"I have an oil fired-furnace using this much oil flow-rate and delivering this much heat to my load. If I substitute the oil with natural gas, will I need more fuel, will my load reach the required process temperature? What flue gas temperatures would I expect?"

We present two representative cases from Collin and dos Santos (1988) which were prepared using the model developed here. Fig. 1 presents the case of a furnace and Fig. 2 the case of a boiler.



Figure 1 Illustrative model results for a furnace.
The model should work well for this case since combustion will be well distributed throughout the boiler. For example, in a tangentially-fired boiler the turbulent ball of fire essentially fills most of the boiler's radiative section. Figure 3 summarizes the results of interest concerning this application. We can arrive at the following conclusions:

- Natural gas, as shown in the examples, can give superior radiative performance than oil for low soot concentrations;
- Soot is only effective to a certain low level after which no increase in performance is seen; and
- 3. Increase in performance might not outweigh maintenance and cleaning/emission control equipment.





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# APPENDIX: USERS' MANUAL

Program Diskette: two directories

EXECUTE CODE

To change to either directory from DOS type:

> cd execute

or

> cd code

(NOTE: any command must be followed by pressing the RETURN key to be executed.)

1. DIRECTORY EXECUTE contains:

\* one executable file

UGN. EXE

TD START THE MODEL the user changes directory to execute and types

) ugn

This executable file has been compiled from FORTRAN. To run the model little help from this manual should be needed: Simply follow the instructions on the screen and very importantly: ENTER THE DIMENSIONS ACCORDING TO FIGURE A.1.

Once the command ugn is entered the user is prompted for input. Each input is followed by pressing the RETURN key. The geometry assumed by the model is as given in Fig. A.1. The user must enter the values accordingly!





As discussed in Chapter 4 of this report, there are seven unknowns:

- One equation for each wall radiative heat balance, for a total of six equations; and
- One equation for the overall conservation of energy between the fuel input and the useful energy absobed by the load and the amount of leaving the radiative enclosure in the flue gases.

The user has to specify the wall boundary conditions. A combination of six unknowns can be handled: each wall will have either a temperature or a total radiative flow. Each unknown is entered as a "1" for a total of six "1s." Fig. A.2 is a copy of how

the screen will typically look for the case of a boiler. Fig. A.3 is a copy of how the screen will look for the case of a furnace.

```
ENTER FUEL:
NATURAL GAS (100% METHANE), (0)
01L NO. 1, (1)
01L NO. 4, (4)
OIL NO. 6, (6)
GASOL, PROPAN 95, (7)
0
    LENGTH OF SIDES, 11-13, m,
665
    WALL EMISSIVITIES, e1-e6
.9.9.9.9.9.9
    ENTER WALL UNKNOWN AS A "1", FOR A TOTAL OF 6 UNKNOWNS FOR Q AND T
    WALL TEMPERATURES , T1~T6, C
200 200 200 200 200 200
    WALL HEAT FLOW, Q1-Q6, MW
1 1 1 1 1 1
    POWER INPUT, NW
60
    EXCESS AIR, %
5
    SOOT CONCENTRATION, g/#3
Ú
    SOOT CONCENTRATION, g/m3
Û
         ITERATION NO.
                        1
         ITERATION NO.
                         2
         ITERATION NO.
                         З
         ITERATION NO. 4
  METHANE POWER INPUT: 60.00 MW
  L1-L3, a: 6.0 6.0 6.0
  wall emiss: .90 .90 .90 .90 .90 .90
  Excess Air (%): 5.0
  Soot Concentration (g/m3): .00
  Wall Temperature T1-T6 (C): 200.0 200.0 200.0 200.0 200.0 Wall Heat Flow Q1-Q6 (MW): 3.997 3.997 3.997 3.997 3.997
                                                                          200.0
                                                                          3.997
  Furnace Radiative Dutput (MW): .240E+02
                                   . 40
  Furnace Radiative Efficiency
  Gas Temperature (C): 1267.4
    WOULD YOU LIKE ANOTER RUN? YES(1), NO(0)
```

Figure A.2 Boiler case.

```
ENTER FUEL:
NATURAL GAS (100% METHANE), (0)
OIL NO. 1, (1)
OIL NO. 4, (4)
OIL NO. 5, (5)
OIL NO. 6, (6)
GASOL, PROPAN 95, (7)
0
      LENGTH OF SIDES, 11-13, m,
626
      WALL EMISSIVITIES, e1-e6
.8 .8 .8 .8 .8
ENTER WALL UNKNOWN AS A "1", FOR A TOTAL OF 6 UNKOWNS FOR Q AND T
      WALL TEMPERATURES , T1-T6, C
1 1 1000 1 1 1
WALL HEAT FLOW, Q1-Q6, MW
0 0 1 0 0 0
POWER INPUT, MW
20
      EXCESS AIR, %
5
      SOOT CONCENTRATION, g/m3
0
             ITERATION NO.
ITERATION NO.
                                   12
              ITERATION NO.
                                    3
              ITERATION NO.
                                    4
              ITERATION NO.
                                   5
    METHANE POWER INPUT:
                                        20.00 MW
   L1-L3, m: 6.0 2.0 6.0
wall emiss: .80 .80 .90
Excess Air (%): 5.0
                                              .80
                                                     .80
                                                             .80
    Soot Concentration (g/m3):
                                               .00
   Wall Temperature T1-T6 (C): 1276.1 1276.1
Wall Heat Flow Q1-Q6 (MW): .000 .000
Furnace Radiative Output (MW): .630E+01
Furnace Radiative Efficiency .32
Gas Temperature (C): 1426.1
                                               1276.1 1276.1 1000.0 1276.1 1256.3 1276.1
                                                                                                             .000
                                                                        6.301
                                                                                     .000
                                                                                                 .000
       WOULD YOU LIKE ANOTER RUN? YES(1), NO(0)
```

Figure A.3 Furnace case.

#### RANGE OF VALIDITY AND CONVERGENCE PROBLEMS

The model attempts a description of reality, therefore, input which does not make physical sense will result in either an error, with interrupt and kick-back to DOS, or in no convergence--the program will run for ever. While the model is runing the ITERATION NUMBER will be displayed. Based on experience after about 20 iterations the program is interrupted automatically since it is assumed it will not converge with further iterations.

The following are typical situations of nonconvergence:

# QFUEL is not enough to heat the wall(s) to the user specified temperature. To correct: increase QFUEL or decrease wall temperatures.

TGAS is too close, order of 10°C, to the wall(s) temperature, this results in oscillation of the gas temperature. To correct: lower wall temperature(s) or increase QFUEL.

The results are questionnable if either P\*L for carbon dioxide or water vapor exceed 5.98. This situation would occur for very long furnaces. It probably will not occur in practice.

Too much fuel is added so TGAS > 2000K. The results are questionable since the correlations for mixture radiative properties are not valid over this limit. (the errors increase and trends could be misleading.)

The following are recommended limits for the input variables:

length: ratio between the largest side and the smallest side to remain as close to one as possible

 $0 \leq \text{soot concentration, } g/s^2 \leq 5$  (?)

Excess air ≥ 0%

 $0.0 \le wall emissivity \le 1.0$ 

200°C ≤ wall temperature ≤ 1700°C

QRAD/FURNACE VOLUME 1.5 MW/m3

Best wishes, "lycka till!" If all fails, the author can be reached at KTH, (OB) 790 8407.

2. DIRECTORY CODE

The directory entitled CODE contains all the code required to assemble UGN.EXE. These subroutines are written in FORTRAN. The compiler used was:

MS-FORTRAN, VERSION 4.0