IMPLEMENTATION OF RADIATION IN ISAT

by

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Abstract

The effects of heat loss due to radiation have been implemented in the ISAT code(for *in situ* adaptive tabulation of combustion chemistry). The simple radiation model is for radiant emission from CO_2, H_2O, CH_4 and CO in the optically-thin limit. The Planck mean absorption coefficients for each species are obtained from the RADCAL program. Two tests are reported to confirm the correct implementation of the model.

Introduction

The use of detailed chemistry in combustion calculations is crucial for the accurate prediction of emissions, ignition, extinction and other performance characteristics that are important from an environmental and industrial viewpoint. A typical reaction mechanism, for example, methane combustion, involves tens of species and hundreds of reactions. In most practical combustion problems there are additional complicating factors such as geometric complexity and turbulence. However, due to the enormous computational expense, a compromise has to be made to handle these complexities and include detailed kinetics.

The *in situ* adaptive tabulation (ISAT) algorithm developed by Pope [2] has significantly alleviated this dilemma and made it possible to economically incorporate detailed chemistry in turbulence combustion calculations.

The current version of ISAT assumes that there is no radiative heat loss. However, for some reaction systems, the prediction of certain species such as nitric oxide (NO), whose production rate is very sensitive to local temperature, may be inaccurate if the effects of radiation are negleted.

In this report, a simple radiation heat transfer model is described. A fortran subroutine based on this model has been added to the ISAT library.

Radiation Model

The thermal radiation model described here is highly simplified based on the following assumptions:

1. the medium is an ideal gas mixture

2. radiant emission is assumed to be solely from the following species: CO_2, H_2O, CH_4 and CO

3. the medium is optically thin

The first assumption implies that there is no soot present. Emission from other species can readily be incorporated if the species mean absorption coefficient is known. The final assumption implies that there is no absorption of radiation by the medium.

Under these assumptions, each radiating point source has an unimpeded isotropic view of the cold surroundings. The radiative heat loss rate per unit volume can be expressed as:

$$Q_r = 4\sigma \sum_{i=1}^{n} (P_i \alpha_{p,i})(T^4 - T_b^4), \tag{1}$$

where $\sigma = 5.669 \times 10^{-8} W/m^2K^4$ is the *Stefan-Boltzmann* constant; P_i is the partial pressure of species i in atmospheres (mole fraction times local pressure in atmosphere); $\alpha_{p,i}$ is the *Planck* mean absorption coefficient of species i; n is the number of species; T is the local flame temperature(K); and T_b is the background temperature.

The *Planck* mean absorption coefficients of CO_2, H_2O, CH_4 and CO are calculated by the **RADCAL** program [1]. Figure 1 shows these coefficients as functions of temperature.

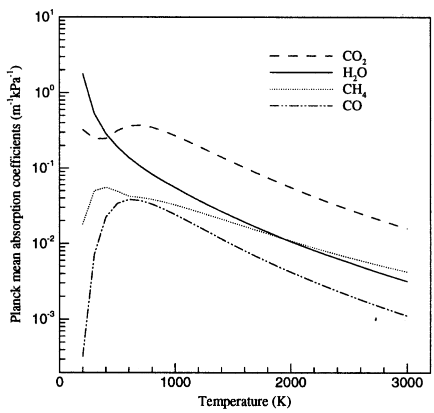

Figure 1: Planck mean absorption coefficients obtained from RADCAL

For a homogeneous, isobaric, adiabatic gas mixture, the specific enthalpy is conserved during reaction. Hence the conservation equations for enthalpy and temperature are

$$\rho \frac{dh}{dt} = 0, \qquad \rho C_p \frac{dT}{dt} = \dot{h}_R,$$

where ρ is the density of the gas mixture; C_p is the constant pressure specific heat; and $\dot{h}_R$ is the source of specific sensible enthalpy due to reaction. Radiative heat loss is incorporated directly by

$$\rho \frac{dh}{dt} = -Q_r, \qquad \rho C_p \frac{dT}{dt} = \dot{h}_R - Q_r. \tag{2}$$

Implementation in ISAT

The implementation of radiative heat loss in ISAT is straightforward, and involves three steps. An overview of the modules and files involved is shown in Figure 2.

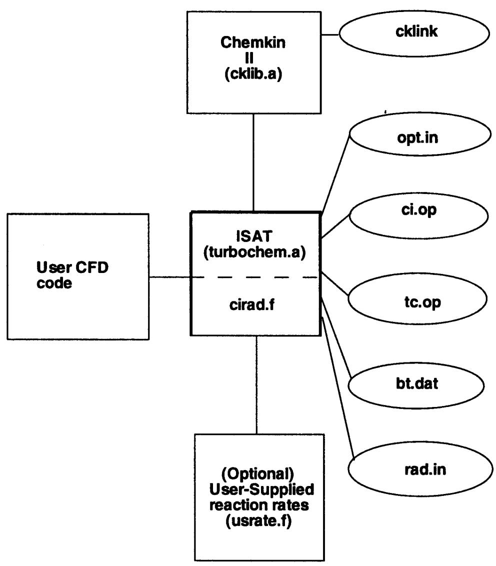

Figure 2: Overview of ISAT modules and files.

Table of Absorption Coefficients

The data file rad.in must be provided. This contains, for each species, a table of the absorption coefficient $\alpha_{p,i}$ as a function of temperature. A typical example of rad.in reads:

```
300.
4
CO2          1.000e+00
H2O          1.000e+00
CH4          1.000e+00
CO           1.000e+00
300.00  0.399E+00  0.168E+01  0.584E-01  0.687E+00
500.00  0.391E+00  0.189E+00  0.481E-01  0.338E+00
... ...
```

where: the first line is the background temperature(T_b); the second line indicates the number of species tabulated(*nrad*); the next *nrad* lines contain the names of the species tabulated and their augmentation factors(*augrad(j)*, explained below); and the subsequent lines make up the table, in which the first column is temperature, and the other columns are absorption coefficients corresponding to the species listed in line 3 through $3 + nrad$ respectivly at the given temperature.

In the evaluation of Q_r by Eq.(1), the absorption coefficient for each species is multiplied by its augmentation factor. Hence, for normal use, each augmentation factor should be set to unity. Sensitivity of the overall calculation to radiation can be explored by changing the augmentation factors. For example, setting the augmentation for a species to zero is equivalent to reflecting its radiation completely.

In the CFD lab at Cornell, the version of rad.in used in this report can be found at ~ qtang/ISAT/radiation/pope.

The absorption coefficients obtained from **RADCAL** are shown in Figure 3, compared to the curve-fit suggested at http://www.ca.sandia.gov/tdf/Workshop/Submodels.html. It has been verified by J. P. Gore(private communication) that the values reported here are correctly obtained from **RADCAL**, and consequently that the curve-fits have shortcomings.

Evaluation of Heat Loss

The new subroutine cirad.f evaluates the radiative heat loss Q_r according to Eq.(1). The mixture state is provided by the calling routine, so that T and P_i can be determined. The quantities $\alpha_{p,i}$ and T_b are obtained from rad.in.

Incorporation of Heat Loss in the Energy Equation

In the existing subroutine cidzdt.f, the heat-loss term Q_r in Eq.(2) is subtracted from the expression for $\rho C_p dT/dt$.

Test cases

To gain confidence in the modified ISAT, a test code independent of cirad.f is developed and combined with the original ISAT without radiation calculation capacity. The test code adopts the same radiation model as we have mentioned in section 2. First we use the original ISAT to determine the state of the mixture and then update the temperature by using the test code. The final results is compared with those of the new version ISAT based on the same initial conditioin. Figure 4 shows the overall procedure of performing the test cases.

Inert Gas Mixture Cooling

The first test case is an inert gas mixture cooling process. Four species are included in the mixture and the mole ratio is $N_2 : O_2 : CO_2 : H_2O = 0.78 : 0.21 : 0.05 : 0.05$. The initial temperature is $2500K$. We assume that the mixture is homogeneous and isobaric, and only the radiative heat loss is considered.

Figure 5 shows the results of the inert gas mixture cooling test. The results match each other exactly.

Autoignition Process

The second test case is an autoignition system. The initial gas mixture consists of methane and air and the mole ratio of species is $N_2 : O_2 : CH_4 = 0.715 : 0.19 : 0.095$. The initial temperature is set to be $1500K$. Again, we assume that the mixture is homogeneous and isobaric, and the heat loss is solely because of the thermal radiation. Specifically, a 19-species methane/air combustion mechanism(ARM2) developed by Sung *et al.*[3] has been used. This mechanism can predict the generation of NO_x which is very sensitive to the local temperature.

Figure 6 shows the temperature profile against time of the autoignition system, and the result of the new ISAT fits the test code result very well.

Conclusions

The ISAT code has been extended to incorporate heat loss due to radiative emission. The absorption coefficients for the species considered(CO_2, H_2O, CH_4, CO) are obtained from **RADCAL**. Two tests have been performed to verify that the implementation is correct.

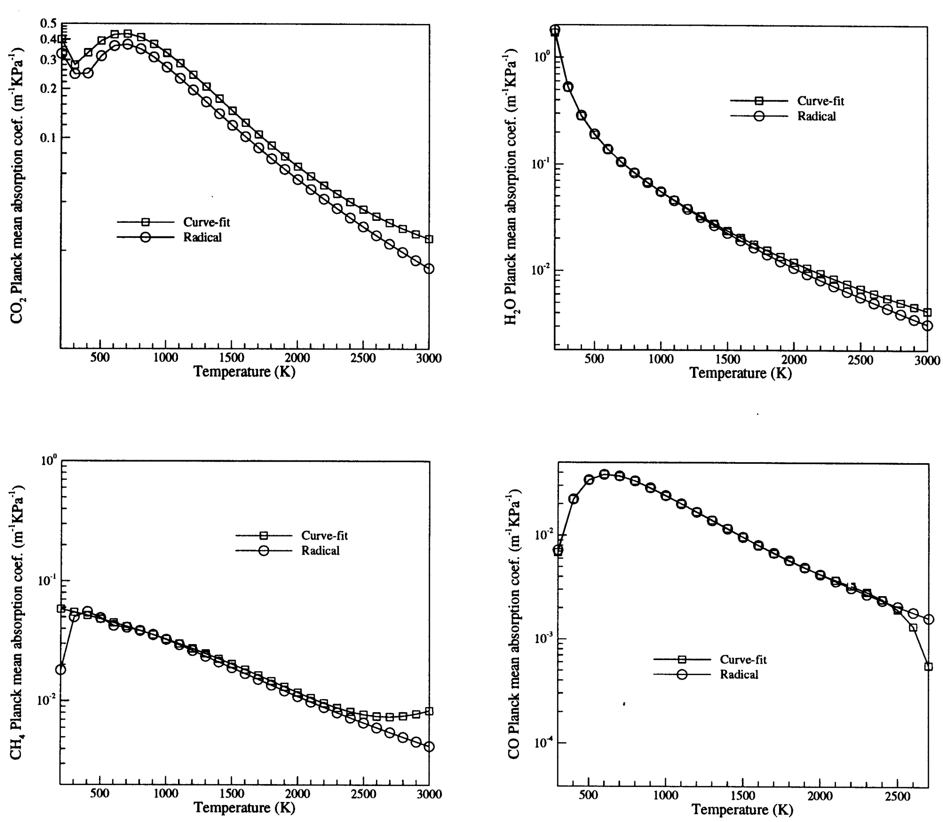

Figure 3: Planck mean absorption coefficient: comparison of value from RADCAL and from curve-fit.

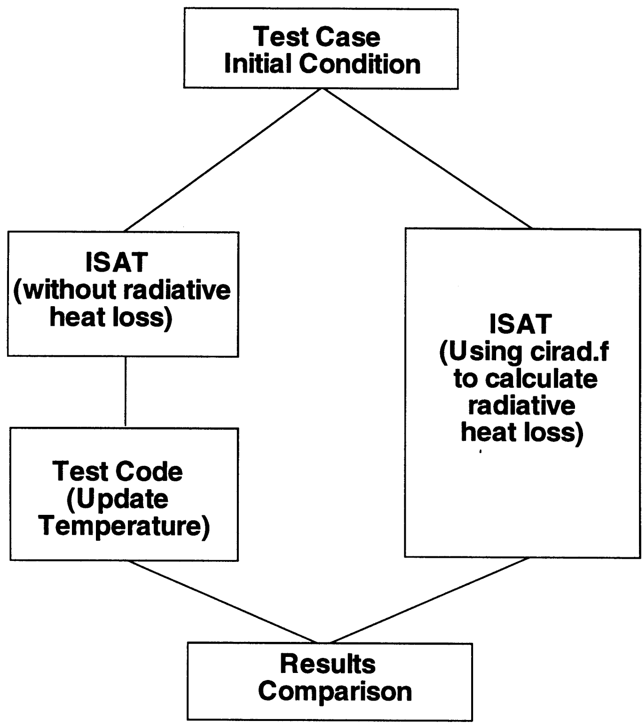

Figure 4: Test code modules

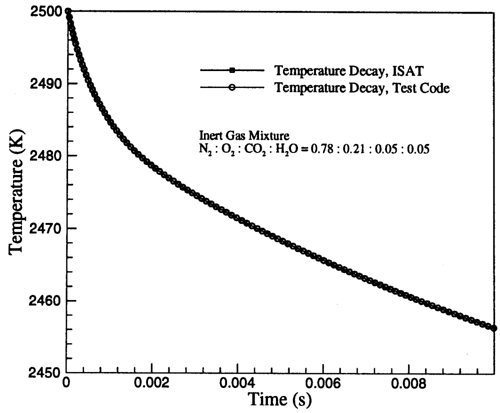

Figure 5: Inert gas mixture cooling.

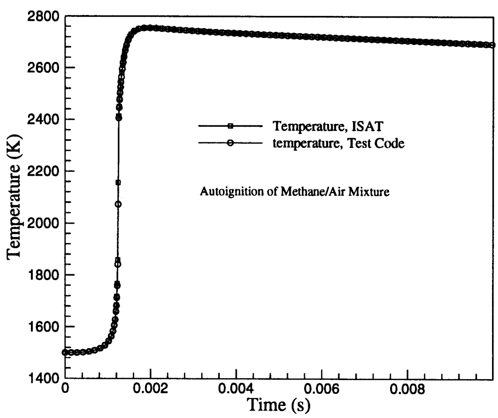

Figure 6: Autoignition test case.

Bibliography

[1] W. L. Grosshandler. *RADCAL: A Narrow-Band Model for Radiation Calculations in a Combustion Environment.* NIST, NIST, Building 224, room B-356, Gaithersburg, MD 20899, USA, 4 1993.

[2] S. B. Pope. Computationally efficient implementation of combustion chemistry using *in situ* adaptive tabulation. *Combust. Theo. Modelling*, 1:41, 1997.

[3] C. J. Sung, C. K. Law, and J.-Y. Chen. An augmented reduced mechanism for methane oxidation with comprehensive global parametric validation. In *Twenty–Fourth Symp. (International) on Combust.*, page 295. The Combustion Institute, 1998.