ROCRAD Developer's Guide

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Title:	ROCRAD Developer's Guide
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Chapter 1

Introduction

1.1 Objectives

The objectives of the radiation module Rocrad is to take account for radiative transfer of heat released from burning aluminum droplets and aluminum oxide continuum particles, and from igniter flame in rocket simulations. In addition, it also considers radiation of emitting, absorbing and scattering particles which may vary in frequency (non-gray).

1.2 Radiation in fluid

Radiation inside solid propellant chamber can be considered as hydrodynamic radiation. For appropriate modeling, we need to understand the effect of radiation in fluid as starting point. The role of radiation in fluid is,

- as additional heat transfer mechanism to the conductive heat transfer in the equation for the rate of change of energy density,
- add radiant energy to the fluid in addition to molecular energy,
- modify fluid pressure tensor due to the present of radiation pressure tensor.

1.3 Assumptions

Simplification of in modeling can be achieved by assuming that the second and third role above are much less dominant than the first. This renders the effect of radiation only appears as a component of rate of heat transfer in the equation of conservation of energy. Further assumption is that we consider only gray gas for now, neglecting the fact that different particles may emit or absorb heat at different frequency. As first model, we assume that the fluid inside propellant chamber is optically thick. This assumption is valid only during steady burning and away from the propellant surface. It is not valid either during the ignition process of solid rocket motor.

1.4 Subroutine organization and compilation procedure

All subroutines pertinent to radiation are placed under directory *rocrad* having name prefix *RADI_*. To activate radiation module user has to include *RADI=1* in the compilation. For instance for structured code, *gmake RFLO=1 RADI MPI=1*

Chapter 2

Formulation

As guided by the physical consideration and assumption above, the physics of radiation heat transfer enters the fluid mechanic equations in the conservation equation of energy density. It can be lumped together with the conductive heat flux rate in the energy equation (see for fluid conservation equations in the developer guide of Rocturb or Rocflo/Rocflu),

$$\partial_t e + ... - \partial_j(-k\partial_j T + q_r) \quad = \quad ... \tag{2.1}$$

with q_r being the radiation heat flux rate (further just called radiation heat flux for brevity), or considered as a source term,

$$\partial_t e + ... - \partial_j(-k\partial_j T) \quad = \quad \partial_j q_r + ... \tag{2.2}$$

We treat the radiation contribution as source term in [*RADI_SourceTerms*] for the sake of better code organization. This results in a higher computational effort compared to lumping it together with the heat conduction term, but the difference is justifiably small.

The key task of radiation module is the computation of q_r, which is related to radiation intensity I by

$$q_r \quad = \quad \int_{\Omega=4\pi} I(\bar{x},\bar{s})d\Omega, \tag{2.3}$$

where Ω is solid angle, $\bar{x}$ is Cartesian coordinate vector, and $\bar{s}$ is vector of incident radiation angle. The integration is thus performed over all possible incident radiation angles (sphere) at each coordinate point. The radiation heat flux can be determined for general condition or optically thick condition. For general condition q_r is derived from its relation to the radiation intensity in Equation (2.3), where the radiation intensity is obtained by solving the following radiative transfer equation (RTE) for each incident direction (Sparrow and Cess 1978),

$$\frac{I(\bar{x},\bar{s})}{d\bar{s}} \quad = \quad KI_b - (K+\gamma)I + \frac{\gamma}{4\pi}\int_{\Omega_i=4\pi} I(\bar{x},\bar{s_i})\phi(\bar{s},\bar{s_i})d\Omega_i, \tag{2.4}$$

with K and γ denoting absorbsion/emission and scattering coefficients, respectively, I_b the black body radiation intensity, and $\phi(\bar{s},\bar{s_i})$ scattering function. The first term represent the black body emission, the second term attenuation due to absorbsion and scattering $\bar{s} \to \bar{s}_i$, and the third term augmentation due to scattering of all $\bar{s}_i \to \bar{s}$. In the current implementation, however, we assume that the medium is optically thick. Under this assumption, q_r can be obtained using diffusion approximation, expressing the radiation flux in a simple algebraic equation,

$$
\begin{aligned}
q_r &= -\frac{4}{3\beta_r}\text{grad}(e_b) && (2.5)\\
&= -\frac{4}{3\beta_r}\text{grad}(\sigma T^4) && (2.6)\\
&= -\frac{4}{3}\frac{4\sigma T^3}{\beta_r}\text{grad}(T) \quad [\mathit{RADI\_DiffRadFlux}, \mathit{RADI\_DiffRadFluxPatch}], && (2.7)
\end{aligned}
$$

where β_r denotes extinction coefficient, a function of medium property, such as particles volume fraction and its computation can be found in [*RADI_ExtinctionCoef*].

Using the diffusion approximation, the local radiation intensity can be expressed as

$$
\begin{aligned}
I(\bar{x}, \bar{s}) &= I_b - \frac{1}{\beta_e \pi}\bar{s}\text{grad}(e_b) && (2.8)\\
&= \frac{\sigma T^4}{\pi} - \frac{4\sigma T^3}{\beta_e \pi}\bar{s}\text{grad}(T) && (2.9)\\
&= \frac{\sigma T^3}{\pi}(T - \frac{4}{\beta_e}\bar{s}\text{grad}(T)) \quad [\mathit{RADI\_DiffRadIntens}], && (2.10)
\end{aligned}
$$

where $\sigma = 5.67\times 10^{-8}\text{W/m}^2\text{K}^4$ is the Stefan-Boltzman constant, prescribed in [*RADI_DerivedInputValues*] and β_e is the equivalent isotropic extinction coefficient of anisotropic medium. In the implementation, we simply use β_r for β_e.

Chapter 3

Code Organization

3.1 Code structure

The task of *rocrad* is to provide the radiation heat flux as a source term in the energy equation. The sequence of computation under diffusion approximation within RK time stepping scheme is first we compute the extinction coefficient in [*RADI_ExtinctionCoef*], then radiation flux q_r is computed in [*RADI_DiffRadFlux*] and [*RADI_DiffRadFluxPatch*], and if desired the intensity can obtained from [*RADI_DiffRadIntens*]. Finally, the divergent of the resulting radiation flux is added as source term in the energy conservation equation through [*RADI_SourceTerms*].

3.2 Data structures

The data structures for the radiation module can be found in the module file *ModRadiation* in directory *modfloflu*. The data pertinent to rocrad user input variables and variables which have only single value per region are declared under type *t_radi_input*. Radiation field variables are declared under type *t_radi*.

3.3 Required input

User input variables and their description can be found in the User Guide of Rocrad.

Bibliography

[1] Sparrow, E.M., and Cess, R.D. (1978). Radiation Heat Transfer, augmented ed., *Hemisphere Publishing Corporation*, Washington.