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Addressing Modeling Requirements for Radiation Heat Transfer

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Abstract

Thermal analysts address a wide variety of applications requiring the simulation of radiation heat transfer phenomena. There are gaps in the currently available modeling capabilities. Addressing these gaps would allow for the consideration of additional physics and increase confidence in simulation predictions. This document outlines a five year plan to address the current and future needs of the analyst community with regards to modeling radiation heat transfer processes. This plan represents a significant multi-year effort that must be supported on an ongoing basis.

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TABLES

NOMENCLATURE

CRT	Capability Realization Team
MBL	Mean Beam Length
NW	Nuclear Weapons
OMD	Organic Material Decomposition
PIRT	Phenomena Identification Ranking Table
PMR	Participating Media Radiation
SPn	Simplified Spherical Harmonics
Sn	Discrete Ordinates

1. INTRODUCTION

Thermal analysts address a wide variety of different applications which involve the simulation of radiation heat transfer phenomena. These applications span wide ranges of parameter values and effective and efficient modeling necessitates a variety of different modeling approaches. There are currently four different modeling approaches presently implemented within SIERRA.

- Exchange factor method (Chapparal)
- Mean beam length (MBL) exchange factor method (Chapparal)
- Discrete ordinates (Sn) method (Syrinx)
- Effective conductivity model (ARIA)

These modeling approaches are varied and each is appropriate for some applications but not all. Chapparal is designed to treat enclosures with diffuse boundaries and transparent or nearly transparent media. It may be applied to non-static geometries but because of large overhead costs static geometries are preferred. Chapparal does not require that the interior of the enclosure be meshed. The effective conductivity model is the most basic participating media solver currently available. Its domain of validity is limited by the fact that it assumes a diffuse intensity and does not incorporate separate boundary conditions for the radiative transfer. As such, it is best applied in highly scattering environments away from boundaries. The discrete ordinates method available in Syrinx is currently the most general radiation modeling capability. It is capable of reproducing the transport equation results in both the optically thin and thick limits. There are certain limitations that are inherent to the discrete ordinates method (ray effects and false scattering) as well as limitations of the current implementation in Syrinx (lack of scalability and non-monotonicity).

The primary goal of the recent capability realization team (CRT) meeting was to assess the current radiation heat transfer modeling capabilities and seek guidance from the analyst community to identify current gaps in our modeling capability as well as additional capabilities that would be most useful. Representatives from the experimental and code development communities were also present to provide input. The information from this meeting was used to develop a phenomena identification ranking table (PIRT) to assist in the planning of future development efforts. A consistent theme was the desire of analysts to have a wider variety of methodologies implemented so as to allow the analyst more freedom in choosing the most appropriate model for a particular application. This desire was shared across all application spaces. A memorandum [1] prepared by Dean Dobranich provides a good discussion of each of the potential methods that might be implemented along with recommendations. Some of those recommendations have already been implemented (MBL) while some remain in progress (simplified spherical harmonics, SPn).

It was emphasized that capabilities that allow us to model additional physics must be accompanied by an experimental effort to define additional property values. This experimental effort could be quite significant considering the large number of different organic materials and gas products present in our systems. In addition, properties may vary based upon material, temperature, time, wavelength, direction, and fouling/oxidation state. There is currently an experimental effort underway to assess the relative importance of these dependencies for the surface emissivity [2]. Preliminary results indicate that the directional dependence is a lower order effect.

There is currently a code development effort underway to implement the SPn method this fiscal year (FY14). Additionally, there is an investigation into the feasibility of coupling with the existing radiation transport code SCEPTRE, which was developed and is maintained by staff in Organization 1300 [3-8]. The analysts expressed a strong interest in the capabilities that SCEPTRE would provide, particularly the spherical harmonics method, highly parallelizable discrete ordinates method, and the capability of treating spectral properties. It was stated that even a partial integration with SCEPTRE would be potentially useful for validation exercises and/or benchmarking. Multiple analysis options provide flexibility and agility for analysts.

2. PHENOMENA IDENTIFICATION RANKING TABLE (PIRT)

There are currently three primary user groups that would benefit from improved radiation heat transfer modeling. Those are the NW internal, fire, and satellite communities. Each group has differing sets of physical phenomena that are relevant to the problems that they solve. Additionally each group may be interested in multiple physical regimes. This is particularly true for NW internal and fire applications where material properties can vary widely based on the temperature, pressure, material concentrations, surface treatments, stages of decomposition, as well as many other factors.

Once the potential physical phenomena were determined, the importance of accurately modeling each phenomenon within various physical regimes to each application area was evaluated. Finally, the adequacy of the current modeling capabilities was determined based on validation exercises. Each modeling capability is marked as either adequate ("A"), inadequate ("I"), or undetermined ("U") (potentially either adequate or inadequate depending upon specific application requirements). The phenomena are labeled with a letter-number pair. The letters in the phenomena numbering scheme correspond to the actual physical phenomena being discussed. The numbers denote the opacity regime being described.

Table 1. Identifying Key Phenomena

	Phenomena	Importance to:			Adequacy
		NW Internal Applications	Fire Applications	Satellite Applications	
Transparent Media	A-1 Spectral Emissivity	High	Low	High	A
	B-1 Diffuse Boundaries	High	High	High	A
	C-1 Non-Diffuse Boundaries (i.e., Specular Surfaces)	Low	Low	Medium	I
Optically Thin Media	D-2 Gray Media	High	High	Low	A
	E-2 Spectral Media	Medium	Medium	Low	I
	F-2 Isotropic Scattering	Medium	Medium	Low	I
	G-2 Anisotropic Scattering	Low	Low	Low	I
	A-2 Spectral Emissivity	High	High	Low	A
	B-2 Diffuse Boundaries	High	High	Low	A
	C-2 Non Diffuse Boundaries	Low	Low	Low	I
Intermediate Optical Thickness Media	D-3 Gray Media	High	High	Low	U
	E-3 Spectral Media	Medium	Medium	Low	I
	F-3 Isotropic Scattering	Medium	Medium	Low	U
	G-3 Anisotropic Scattering	Low	Low	Low	I
	A-3 Spectral Emissivity	High	High	Low	I
	B-3 Diffuse Boundaries	High	High	Low	U
	C-3 Non Diffuse Boundaries	Low	Low	Low	I
Optically Thick Media	D-4 Gray Media	High	High	Low	U
	E-4 Spectral Media	Medium	Medium	Low	I
	F-4 Isotropic Scattering	Medium	Medium	Low	U
	G-4 Anisotropic Scattering	Low	Low	Low	I
	A-4 Spectral Emissivity	High	High	Low	I
	B-4 Diffuse Boundaries	High	High	Low	I
	C-4 Non Diffuse Boundaries	Low	Low	Low	I

3. EXPLANATION OF PIRT

The numerals in the phenomena numbering scheme designate the opacity regime in which the phenomena occurs. The opacity (or in its non-dimensional form the optical thickness) is a very important parameter in determining the appropriate method for evaluating the radiative heat transfer. It should be noted that in some applications (NW internal and fire) that a wide range of opacity values may be present even within the same problem. In these cases, either the problem must be decomposed in such a way as to allow the coupling or multiple solution methods or a widely applicable method that is valid across the entire range of opacities present must be utilized.

1. Transparent media

Enclosure or surface-to-surface radiative heat transfer often occurs with transparent media. In this situation, there is no emission, attenuation, or scattering from within the volume of the enclosure or between the surfaces. Generally, the cavity does not need to be meshed. The exchange factor method implemented in Chapparal performs well in this regime as long as the boundaries may be accurately assumed to be diffuse. There is a large initial overhead cost associated with inverting the view factor matrix. This can make this method less than ideal for cases with moving meshes or element death since this inversion must be performed repeatedly rather than once.

2. Optically thin media

Optically thin media participates to a small but non-negligible degree. In this regime surface-to-surface transfer remains the dominant mode for radiative exchange but the intervening media does affect the radiative heat transfer. The mean beam length method recently implemented in Chapparal performs well in this regime with a few limiting assumptions such as that of diffusely emitting and reflecting surfaces. The temperature and radiative properties of the medium must be able to be reasonably approximated as gray and uniform. Additionally, the presence of scattering is not well accounted for.

3. Intermediate optical thickness media

Intermediate optical thickness media is a catch-all that covers everything in between the optically thin and optically thick limits. The precise bounds of this regime are nebulous and methods that are valid for intermediate optical thicknesses often remain valid (although computationally inefficient) for optically thin and optically thick media as well. The discrete ordinates method implementation in Syrinx is currently the only capability valid within this regime. Due to limitations inherent to the current implementation there are limits to the size of problem and the number of processors that may be used that may make this capability inadequate for some applications. The discrete ordinates method, by its nature, also introduces spurious oscillations into the solution that can cause hot spots on combustible surfaces and significantly alter results. The presence of these "ray effects" does not depend upon the implementation but is an artifact of the angular (not spatial) discretization. It is possible for the user to increase the resolution of the angular discretization in order to mitigate the "ray effects" albeit at great computational expense.

4. Optically thick media

Optically thick media is defined such that the mean-free-path of photons traversing the domain is small relative to a characteristic dimension of that domain. There are a number of approximations that may be made when the medium is optically thick that greatly accelerates solution times. In the optically thick regime, special attention must be paid to the scattering albedo since the applicability of many optically thick approximations is dependent upon the presence of a relatively isotropic intensity. This assumption is valid for highly scattering media but is likely invalid for purely absorbing media. Low order spherical harmonics expansions rely upon this assumption, for example. The effective conductivity model available in ARIA is the only current capability for evaluating radiative transport in optically thick media. Unfortunately, the effective conductivity model is not always valid near boundaries and a "jump coefficient" must be used to accurately model the boundary. This "jump coefficient" is not currently available in ARIA and thus the effective conductivity model may be inadequate for certain applications for which this discrepancy is important. It has been noted that the effective conductivity model performs well when modeling high-char foams but less well when foam decomposition leaves a significant void region. In these situations, the underlying assumptions of the method are violated. The discrete ordinates method in Syrinx is technically valid in this regime, but the discrete ordinates method tends to suffer from extreme ray-effects and reduced accuracy in optically thick purely absorbing applications.

The letters in the phenomena numbering scheme correspond to the actual physical phenomena being discussed. These phenomena may be present in multiple opacity regimes and their relative importance may change as a function of optical thickness, application space, and other factors.

A. Spectral emissivity

Spectral emissivity refers to the dependence of surface properties on wavelength. For most real surfaces the emissivity and reflectivity are somewhat strong functions of the wavelength of the incident radiation. Currently, the exchange factor method in Chapparal is the only capability for including spectral emissivity in a model. Chapparal allows for banded (piecewise constant) emissivities. It is difficult to accurately measure spectral radiative properties. Also, these properties can change during a heating event due to surface alterations such as oxidation and fouling. Computational and experimental investigations are needed to explore the materials and conditions for which spectral properties are needed for accurate thermal models.

B. Diffuse boundaries

Diffuse boundaries assume that emission from a surface and reflection off of a surface are both independent of direction. This is a reasonably good approximation for a wide range of engineering materials. This assumption is made in the implementation of all current radiation heat transfer capabilities with the exception of the effective conductivity model which does not include boundary conditions.

C. Non-diffuse boundaries

Non-diffuse boundaries (a.k.a., specular surfaces) are ones for which the previously described assumption of diffuse boundaries is invalid. These may include textured surfaces or highly polished surfaces. In these cases, the emissivity may vary with direction and the reflectivity may vary with both the angle of incidence and the angle of reflection. There is no current capability for treating non-diffuse boundaries within the SIERRA codes. Techniques exist in the literature for measuring bidirectional reflectances, but there is currently no experimental effort targeted towards making these measurements for relevant materials. Some measurements have been made for specialized surfaces that were textured to tailor the directionality of the reflected radiation.

D. Gray media

Gray media refers to the assumption that the optical properties of the medium are independent of wavelength. This is generally a poor assumption for most gases as they tend to have spectral bands that are both optically thick and optically thin. However, the assumption may be justified for certain applications where the radiation effects are less important or when the optical thickness is sufficiently small or the medium properties are nearly independent of wavelength within a wavelength range or interest. The assumption is also currently required as it is inherent to the implementation of all radiative heat transfer capabilities within the SIERRA codes. The distinction between the assumption of gray media and the assumption of gray surface emissivity is emphasized.

E. Spectral media

Spectral media refers to relaxing the gray media assumption and allowing some or all of the optical properties to vary with wavelength. There are a number of different models for including spectral media that each have pros and cons. Most of them are structured in such a way that they can be implemented in the form of a multi-group approximation. From a computational standpoint, this amounts to discretizing the wavelength space of the radiation. The highly irregular behavior of optical properties as a function of wavelength for many common materials makes this a challenging problem. There are currently no capabilities for treating spectral media within the SIERRA codes.

F. Isotropic scattering

Isotropic scattering is the simplest implementation of scattering phenomena. The direction that a photon scatters into is assumed to be independent of the direction the photon was traveling prior to the scattering event. This is a very common engineering approximation and is valid for many applications. Currently, the discrete ordinates method implemented in Syrinx is capable of evaluating radiative heat transfer in the presence of isotropic scattering. The simplified spherical harmonics method implementation currently being developed for ARIA is also capable of treating isotropic scattering.

G. Anisotropic scattering

Anisotropic scattering refers to more general treatment of radiative scattering. Isotropic scattering may be seen as a subset of more general anisotropic scattering theory. In general, scattering phenomena are anisotropic. However, the impact of this anisotropy is considered to be relatively small for many of the applications of interest. Often, even if treatment of scattering as isotropic is inadequate, treatment of scattering as linearly anisotropic is sufficient. There are currently no capabilities within the SIERRA codes for treating anisotropic scattering.

4. SUMMARY OF OTHER CRT COMMENTS

In addition to the phenomena ranking, the following points of emphasis were made. These are in no particular order but seem to reflect the priorities of the analyst community with regards to future participating media radiative heat transfer model development.

- The capability of modeling additional physics must be accompanied by appropriate experimental investigations.
- The commitment to continued maintenance and support of software capabilities beyond the development phase is crucial.
- Any additional modeling capabilities would be appreciated although there is a trade-off between implementation cost and utility that must be considered.
- A wide variety of methodologies would be best so as to allow the analyst more agility when juggling model fidelity and solution time constraints.
- The availability of additional tools will necessitate the development of a knowledgebase of when each is appropriate.
- Currently, radiation heat transfer models have had little or no V&V in the last 15 years and past V&V effort has been concentrated on enclosure radiation or coupled physics in fire environments [9-11]. There is a lack of quality participating media datasets where radiative heat transfer is the dominant physics.
- Consolidated documentation of current radiation models as well as any additional radiation models implemented would be valuable.
- Models to predict the evolution of surface emissivity due to the deposition of soot, propellants, and condensable volatiles would be widely applicable.

5. FIVE YEAR PLAN

The following plan provides a roadmap to meet the participating media radiation needs over the next five years. This plan represents a significant level of effort that must be supported over several years.

FY14

- Implement simplified spherical harmonics (SPn) approximation for PMR in ARIA. This capability should be available natively for ARIA users and through transfers to Fuego users (similar to how Syrinx is currently coupled to Fuego).
- Conduct surface emissivity experiments. Surface emissivity is a major driver of uncertainty in many NW applications. The time evolution of surface emissivity due to the deposition of soot, propellants, and condensable volatiles is currently poorly understood / modeled.

FY15

- Perform code verification of SPn implementation in ARIA. This should include MMS tests as well as comparisons to Syrinx results for pure radiation and radiation coupled with conduction and/or convection. In particular, coupling with Fuego should be rigorously tested.
- Document SPn usage and verification for the SPn implementation.
- Conduct enclosure radiation validation experiments. Preliminary planning for these experiments was performed in FY14.
- Continue surface emissivity experiments from FY14.

FY16

- Couple SCEPTRE and SIERRA codes. This should provide SIERRA users with access to all relevant SCEPTRE capabilities including a highly scalable implementation of the discrete ordinates method, as well as a finite element in angle method and spherical harmonics methods. All SCEPTRE solution methods are capable of including non-gray (spectral) media, anisotropic scattering, and specular boundary conditions.
- Perform verification of SCEPTRE coupling. SCEPTRE already has a suite of solution verification and regression tests. The coupling verification tests would likely consist of the same problems used to verify the Fuego/ARIA coupling for SPn.
- Document SCEPTRE coupling and usage in SIERRA tools. Additionally, provide SIERRA users with access to existing SCEPTRE documentation [12].
- Design PMR validation experiments. These experiments should span parameter regimes of interest and include relevant multi-physics coupling.
- Conduct literature review and survey of currently available relevant optical property data. In cases where optical property data is not well characterized or unavailable, design and propose experiments to determine the relevant optical properties.

FY17

- Perform PMR validation experiments proposed in FY16.
- Perform parameter studies to assess the validity of various PMR solution methods for different problems of interest such as those involving organic material decomposition (OMD) and sooty or clean-burning fires. This study should address the competing interests of solution accuracy and computational expense and provide analysts with recommendations for which radiation heat transfer models are likely to be appropriate for a given application.
- Design optical property determination experiments proposed in FY16. Depending upon the number and type of properties to be determined and the number of materials to be tested, this could potentially become a large experimental effort.

FY18

- Perform optical property determination experiments proposed in FY16 and designed in FY17.
- Consolidate relevant optical property data from literature (HITRAN etc.) and optical property determination experiments (ongoing in FY18) into a database that is accessible to SIERRA tools. This will ensure that consistent optical property data is available to be used across simulations and that all data is appropriately sourced and documented.

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