

RadLib: a radiative heat transfer model library for CFD

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Abstract

Ca. 100 words

Keywords: radiative heat transfer, reacting flows, CFD

Required Metadata

Current code version

Ancillary data table required for subversion of the codebase. Kindly replace examples in right column with the correct information about your current code, and leave the left column as it is.

Nr.	Code metadata description	Please fill in this column
C1	Current code version	TODO 2.1
C2	Permanent link to code/repository used for this code version	<i>github.com/BYUignite/RadLib</i>
C3	Code Ocean compute capsule	N/A
C4	Legal Code License	MIT license (MIT)
C5	Code versioning system used	Git
C6	Software code languages, tools, and services used	C++, Python 3
C7	Compilation requirements, operating environments & dependencies	TODO
C8	If available Link to developer documentation/manual	TODO
C9	Support email for questions	davidlignell@byu.edu

Table 1: Code metadata (mandatory)

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1. Motivation and significance

Why did we make this? Radiation is hard to deal with in CFD. It's complicated. You can't really get analytic solutions to practical problems. In lots of cases, that's fine because radiation can be safely neglected; it's not usually the dominant mode of heat transfer. However, we do combustion CFD. Radiation isn't always important to combustion problems, but when it is, simulations can get grossly inaccurate. So we need a nice way to account for radiation in our CFD simulations.

When is radiation important to combustion simulations? In high-temperature systems, radiation can often be neglected in the beginning and middle of the simulation (assuming, say, a jet flame or a counterflow flame or something like that). At those times (which I'm going to call "early flame"), convective heat transfer dominates pretty heavily. However, radiation becomes more important for late-stage flame phenomena, either after some time has gone by (radiation time scales?), or physically high up in a flame where convection doesn't dominate as much as below, or just in areas that are relatively far away from the flame sheet itself where the reactions are happening. There's also soot, which involves radiation heavily, but soot particles are so big and slow that their time and length scales (and their radiative time scales) mean that radiation doesn't become important until late in the flame evolution.

So what's the problem? Why hasn't this been done already? Radiation is complicated. So is combustion. Combustion in particular can be so complex that direct simulations are too computationally expensive for us to simulate configurations that are practical for engineering systems. Direct simulations are usually used as a research tool. Other modeling approaches exist (LES, ODT, etc.) that lower the computational cost and allow us to simulate practical things. So far so good.

Radiation is a little like combustion in that its core mechanisms are complex, physically and mathematically. In addition, it's directional AND depends on the wavelength of the energy involved (other heat transfer doesn't have the wavelength dependence); its governing equations integrate over direction and wavelength, which makes things extra complicated. RADIATION GOVERNING EQUATIONS HERE. Convective heat transfer follows easy rules, but radiation doesn't. There are simple systems in which we can boil things down to analytic solutions, but most of the time, the simple equations don't apply, and that's often true in combustion systems where there are so many different length and time scales involved. The fundamental equations of radiative heat transfer are big and mathematically complex; they don't have analytic solutions except in the simplest geometries. So what do we do? One of two things. One, we do ray tracing (sometimes referred

41 to as Monte Carlo simulations. These can be extremely accurate, but super
42 computationally expensive. Essentially the equivalent of a direct numerical
43 solution. Two, we simplify the the equations. We make assumptions. And
44 so on. This is potentially less accurate, but more practical. By simplifying
45 the fundamental governing equations, we create models that apply to various
46 situations, systems, and geometries (i.e. black body assumptions, directional
47 assumptions, etc.). There are models developed for CFD and specific com-
48 bustion systems. These are the models that we've put into practice here in
49 such a way that they're easy to apply to various systems. Modular organi-
50 zation for this purpose.

51 So far there isn't an easy way to access and use radiation models. There
52 are simple ones in Cantera (check this, there might not be any), but they
53 make too many assumptions or don't work well for combustion or what have
54 you. RadLib is a radiation library of models that you can apply to any
55 simulation type, and we'd like to add it to Cantera, too. Basically, there
56 isn't a reliable way to do radiation calculations in CFD simulations without
57 coding the models yourself, which is extra hard because they're complicated
58 and hard. So we've done it for you and put them in a library that easy for
59 anyone to use.

60 Models we're using:

- 61 • planck mean (optically thin?) with coefficients from TNF website [1]
 - 62 – other references from TNF website: [2, 3, 4, 5]
- 63 • weighted sum of grey gases [6, 7]
- 64 • RCSLW model [8]
 - 65 – SLW model [9]
 - 66 – LCSLW [10]
 - 67 – "It is shown that the Rank Correlated SLW model is the most
68 robust of all models, and demonstrates that it can achieve accurate
69 solutions with as few as 3–5 gray gases." [11]

70 Discuss pros and cons of each model for combustion simulations? You still
71 have to pick the right one for your simulation and situation. That discussion
72 might fit better in software description section. See example section for
73 comparisons of models.

74 2. Software description

75 2.1. Model descriptions

76 RadLib includes three models of varying complexity and accuracy to cal-
77 culate the radiation absorption coefficients and their weighting factors for
78 each gas considered by the model. Radiation absorption coefficients are typ-
79 ically calculated using correlations relating them local properties such as
80 temperature, total pressure, or species partial pressure, depending on the
81 model. Correlations come from curve fits to high-resolution radiation prop-
82 erty databases. At present, RadLib considers up to four gas species (H_2O ,
83 CO , CO_2 , and CH_4) and, optionally, soot volume fraction in its calculation
84 of absorption coefficients and weighting factors.

85 Once the radiative absorption coefficients are calculated, they are then
86 used to solve the radiative transfer equation (RTE), which depends on the
87 simulation configuration and assumptions. Solving the RTE is not the focus
88 of this software, but RadLib’s example cases do employ a simple implicit
89 trapezoid method solver to calculate the radiative heat flux and volumetric
90 heat source profiles between two parallel planes. [MORE DESCRIPTION
91 OF SOLVER GOES HERE?]

92 [OTHER THINGS THAT APPLY TO ALL MODELS GO HERE]

93 [MAYBE INCLUDE SOME BASIC INFO ON LBL?]

94 2.1.1. Planck Mean absorption coefficients

95 When we refer to the Planck Mean model, what we’re using is actually the
96 Planck Mean absorption coefficients, calculated from the correlations given
97 on the TNF workshop site [1]. Their correlations (temperature dependent)
98 are based on the RADCAL model in [2]. The TNF radiation model is also
99 documented in [5].

100 This model is commonly used because it’s relatively simple, easy to im-
101 plement, low in computational expense, and provides reasonably accurate
102 results in many cases.

103 Quote from TNF site page: ”The characteristics of some flames selected
104 for the workshop are such that a model based upon the assumption of op-
105 tically thin radiative heat loss should yield reasonable accuracy. This has
106 been demonstrated for the simple hydrogen jet flames [12]. However, there is
107 some evidence that the optically thin model significantly over predicts radi-
108 ative losses from the CH_4 flames in the TNF library, due to strong absorption
109 by the 4.3-micron band of CO_2 [3, 4?].” Basically, it works well for flames
110 that are actually optically thin, but not so well for flames that aren’t. This
111 is especially true of sooting flames.

112 2.1.2. Weighted sum of gray gases (WSGG)

113 The basic assumption of weighted sum of gray gases (WSGG) models
 114 in general is that the non-gray behavior of gas mixtures, in this case H₂O
 115 and CO₂, can be modeled by a weighted sum of several gray gases and one
 116 transparent gas (which represents the spectral windows between absorption
 117 bands). RadLib uses the WSGG model presented by Bordbar et al. [6, 7],
 118 which uses correlations based on the HITEMP 2010 database [13]. RadLib,
 119 in accordance with the Bordbar et al. WSGG method cited above, uses a
 120 mixture of four gray gases and one transparent gas. Absorption coefficients
 121 are calculated by

$$K_i = \sum_{k=0}^4 d_{i,k} M_r^k, \quad (1)$$

122 where K_i is the absorption coefficient for species i , $d_{i,k}$ is a species-specific
 123 correlated model coefficient, and M_r is the molar ratio $Y_{\text{H}_2\text{O}}/Y_{\text{CO}_2}$. The
 124 weight factors are calculated by

$$a_i = \sum_{j=0}^4 b_{i,j} T_r^j, \quad (2)$$

125 where a_i is the weighting factor for species i and T_r is a normalized tem-
 126 perature equal to T/T_{ref} with $T_{ref} = 1200\text{K}$. The value of $b_{i,j}$ is calculated
 127 by

$$b_{i,j} = \sum_{k=0}^4 C_{i,j} M_r^k, \quad (3)$$

128 where $C_{i,j}$ is another correlated model coefficient and M_r is the molar ratio
 129 $Y_{\text{H}_2\text{O}}/Y_{\text{CO}_2}$ as above.

130 2.1.3. Rank Correlated SLW (RCSLW) model

131 2.2. Software Architecture

132 RadLib is an object-oriented C++ class library.

133 Examples folder contains sample driver scripts for using the library.

134 Python version somewhere? Corresponding examples?

135 3. Illustrative Examples

136 Simple comparisons of each of these models to some ray-tracing results
 137 (equivalent to a direct numerical solution) to establish validity. Illustrates
 138 when to use various models and why you might choose one over another.
 139 Plots and discussion go here. Five example cases demonstrated with this code
 140 in both C++ and Python. Compared to line-by-line calculations (essentially
 141 the radiation version of Monte Carlo).

142 4. Impact

143 As far as I'm aware, there isn't an easy way to incorporate radiative heat
144 transfer into a CFD simulation. Most cases use optically thin assumption
145 (which works in some cases, but not in others) or neglect radiation entirely
146 (also applicable sometimes, but not always). [Refer to TNF website radia-
147 tion page here.] Unfortunately, this means that when you simulation some
148 configuration in which radiation might be important to the overall heat trans-
149 fer, you won't get accurate simulation results. Furthermore, if your study is
150 about something else entirely, your radiation model (or lack thereof) becomes
151 a source of error that may be very difficult to separate from other sources of
152 error in your simulation study (i.e. soot modeling studies). As of right now,
153 if you want any detailed radiation treatment, you have to code it yourself,
154 which is difficult and requires external validation.

155 RadLib can make researchers' lives easier by providing a library of preval-
156 idated radiation models that can be switched out with no difficulty. Addi-
157 tional models can be added easily using the provided modular framework.
158 Researchers can even use Radlib as a tool for comparing models. No need
159 to code multiple different complex radiation models yourself just to decide
160 which one works best for your simulation. And no need to puzzle through
161 the literature to figure out which model(s) might be best for your simula-
162 tion, either; instead, you can test them yourself. It saves tons of time and
163 effort that researchers can now put toward results rather than code or model
164 development.

165 By putting all these models side by side in a modular framework, RadLib
166 also provides a structure on which new or altered radiation models can be
167 tested against existing ones. Maybe more comparative studies can be done,
168 especially for more complex simulation cases. We plan to add radiation
169 models as appropriate to RadLib, too.

170 RadLib opens up new horizons for CFD simulations, especially in combus-
171 tion cases. It is designed such that it can be easily incorporated into existing
172 research codes. Our group plans to use it with ODT [CITE OTHER SOFT-
173 WAREX PAPER HERE?] alongside soot model library (in development) to
174 study late-flame phenomena such as soot oxidation, flame extinction, and
175 soot-flame breakthrough. These topics in particular are difficult because
176 they require accurate simulation data over a relatively long computational
177 time in addition to good models for both soot chemistry (which is an active
178 research area) and radiation heat transfer (which is the difficult part that
179 RadLib can solve). Using RadLib for such studies allows us to separate and
180 quantify sources of error that may occur due to various models, which is
181 super difficult if you only have one model to work with or it hasn't been

182 validated well.

183 RadLib can also be used outside of combustion CFD research for anything
184 involving radiative heat transfer. Potential research areas that could benefit
185 include atmospheric and climate sciences, interstellar phenomena, improving
186 efficiency of energy-producing processes, safety in chemical plant design, etc.
187 We aren't experts in these areas, but radiative heat transfer is a universal
188 phenomena that applies to any system or process that involves heat transfer.

189 This software has not been used outside of the current research group,
190 and it is not used in any commercial settings at this time.

191 5. Conclusions

192 Set out the conclusion of this original software publication.

193 6. Conflict of Interest

194 We wish to confirm that there are no known conflicts of interest associated
195 with this publication and there has been no significant financial support for
196 this work that could have influenced its outcome.

197 Acknowledgements

198 The authors extend special thanks to Hadi Bordbar for assistance with
199 the WSGG model and to Vladimir Solovjov and Brent Webb of Brigham
200 Young University for their insights and assistance with the RCSLW model.

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Current executable software version

Ancillary data table required for sub version of the executable software: (x.1, x.2 etc.) kindly replace examples in right column with the correct information about your executables, and leave the left column as it is.

Nr.	(Executable) software meta-data description	Please fill in this column
S1	Current software version	TODO 2.1
S2	Permanent link to executables of this version	TODO For example: https://github.com/combogenomics/DuctApe/releases/tag/DuctApe-0.16.4
S3	Legal Software License	MIT license (MIT)
S4	Computing platforms/Operating Systems	Linux, OS X, Microsoft Windows
S5	Installation requirements & dependencies	TODO
S6	If available, link to user manual - if formally published include a reference to the publication in the reference list	TODO For example: http://mozart.github.io/documentation/
S7	Support email for questions	davidlignell@byu.edu

Table 2: Software metadata (optional)