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RadLib: a radiative heat transfer model library for CFD

--Manuscript Draft--

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Abstract:	RadLib is a C++ library of radiation property models that can be applied to variety of systems involving radiative heat transfer, including CFD simulations. RadLib includes three major radiation property models—Planck Mean (PM) absorption coefficients, the weighted sum of gray gases (WSGG) model, and the rank-correlation spectral line weighted-sum-of-gray-gases (RCSLW) model. RadLib includes C++, Python, and Fortran interfaces and can be expanded to include additional models.Several example cases illustrate the use of the models with an included ray-tracing solver and compare them in terms of accuracy relative to line-by-line solutions. A CFD example is provided of an ethylene burner in a compartment using Fire Dynamics Simulator (FDS). The computational cost of the models is compared. RadLib provides researchers with convenient access to validated radiation property models and a framework for further development.

Cover Letter

CHEMICAL ENGINEERING DEPARTMENT
IRA A. FULTON COLLEGE OF ENGINEERING

July 24, 2021

Andrew Hazel,
Principal Editor
Computer Physics Communications

Dear Professor Hazel:

Please accept the following revision to our paper RaLib: a radiative property model library for CFD, submission COMPHY-D-21-00015R1. The three reviewers had a number of constructive criticisms of the paper and we have made a good-faith effort to modify the paper and code accordingly. A major revision of both was undertaken. In particular, the manuscript increased from 21 to 29 pages and most sections were heavily edited. A Fortran code interface was added alongside the C++ and Python interfaces. We coupled the code to the NIST Fire Dynamics Simulator (FDS) and ran a sample simulation. The build process and documentation were also improved. Around 60 commits were made to the git repository. An updated version of the installation and use example video is provided on youtube. We have also submitted a revised Code Ocean capsule. I appreciate your consideration.

Sincerely,

David O. Lignell
J.J. Christiansen Professor, Associate Chair
Chemical Engineering Department
Brigham Young University

Response to Reviewers: CPC initial submission

Note, reviewer comments are included with responses in blue text.

Reviewer 1

This manuscript introduces "RadLib," a C++ library to calculate absorption coefficients for use in radiative heat transfer calculations. The library has reasonable value to the research community, despite a few limitations in its scope and design. The library is self-contained (doesn't have any external dependencies), which is convenient.

I have a number of comments on the manuscript as well as the software itself which the authors should consider to improve the manuscript and software.

The authors thank the reviewer for their time and careful review.

Manuscript:

1. There is no general user documentation provided in section 3. Figure 1 includes information that is more algorithmic than illustrative of the API.

   Section 3 has been significantly revised and extended to include more information on how users can include and interact with the RadLib library. This includes a description of the build procedure and a list of installed files. Compilation of user code with RadLib is outlined. A description of the interface functions is also provided. The key interface function was `get_k_a(...)`. An additional function is now included and described, `get_k_a_oneband(...)`. The function arguments are now described. Since the initial submission, a Fortran 90 interface has been added and this is included in the section.

2. Section 5 makes several editorial claims that are quite subjective, and not well-supported:

   i. First sentence: "historically difficult to implement … complexity and high computational costs"

      - Property evaluation is not the expensive part of a radiation calculation. Solving the RTE is the expensive part.
        - I wouldn't characterize the property evaluation as particularly complex in comparison with other aspects of combustion simulations (kinetics, thermodynamics, transport properties).

   ii. At the end of the first paragraph, the authors seem to imply that RadLib will solve the challenges of radiation modeling. Again, it is the RTE solver, not the property evaluation, that is the largest time-sink in terms of computer and human resources.

iii. These kinds of statements persist throughout the second paragraph as well. There are limitations in RadLib such as lack of scattering treatment for particle-laden flows, inability to include more species, lack of any line-by-line capabilities, etc. The library checks a few useful boxes, but the verbiage here seems to take more credit than the authors may be due.

In the first sentence and paragraph of Section 5, "radiative heat transfer models" does not refer specifically to either radiation property models or RTE evaluation methods, but the treatment of computational radiative heat transfer as a whole. This generalization was intended for the entire first paragraph of Section 5.

Regarding solution of the RTE versus the radiative property model, the reviewer is correct that in most engineering calculations, specification and implementation of the RTE can be more complex and costly than that of the property model. For both parts, however, this depends strongly on the particular model used, (and the geometry considered). The optically-thin model RTE model is trivial, and the RCSLW property model is not. We revised the manuscript to include a discussion of this in the second paragraph of the introduction, with a specific note that "In practical engineering simulations, the solution of the RTE is often the most complex and costly part of radiative simulation…" That said, we believe that access to good radiative property models as presented in this paper is a valuable contribution.

We want to be careful with what is claimed in the paper, and some major revision has occurred in response to this reviewer's comments and others. Section 4 contained examples provided along with results, but now contains a description of the examples provided with the code. Section 5 contained some discussion items as noted by the reviewer, but now includes simulation results for the examples along with a CFD demonstration. The discussion items noted by the reviewer have been modified and folded into the Conclusions section.

3. Section 5 claims that "RadLib's modular framework is designed to easily accommodate new models as well," which is a bit of an overstatement. See comments below w.r.t. assumptions on species considered, hard-coded polynomial coefficients, etc. all of which reduce extensibility.

   We remove the word "modular" throughout the paper. We do believe that the library can be extended, and have noted this, with softer language, in the revision. The reviewer is correct that we do not provide explicit functionality, for, e.g., generic extension to other species. In some cases, like the PM model, such extension would be trivial within the existing code structure. In the RCSLW model, extension to other species would require provision of the species ALBDF (not trivial), and then extension would be a straightforward, but the code is not set up for arbitrary species in arbitrary order. The library is primarily targeted at combustion applications where CO2 and H2O are the primary radiative species. Future efforts may motivate further extension.

4. There are several minor issues that need to be addressed:

i. Abstract: “well-written” is subjective and should be removed.

Done.

ii. Introduction: second sentence: “Combustion simulations…” is a run-on sentence.

We have revised the wording in the introduction.

iii. Page 10: “[INSERT RUNTIME COMPARISONS HERE]”

This has been corrected.

iv. Section 7 heading: “Interes”

This has been corrected.

Software deficiencies & suggestions:

1. API doxygen documentation is non-standard. It appears that the doxygen documentation is provided in the .cc files rather than the header files, which is where it is typically found. Downstream developers would typically be working from headers and the installed library, so it is convention to have doxygen documentation in the header only. This also reduces clutter in the implementation files.

   We believe this to be a stylistic preference. Here’s a quote from the ***doxygen website***: “Unlike most other documentation systems, doxygen also allows you to put the documentation of members (including global functions) in front of the definition. This way the documentation can be placed in the source file instead of the header file. This keeps the header file compact, and allows the implementer of the members more direct access to the documentation.” Furthermore, Doxygen is primarily used to build external documentation (html), so, from that perspective, it does not seem as important where the Doxygen comments are in the source code. The reviewer’s argument makes more sense for libraries that are distributed without the source. In our case, we provide the source and the header files. We follow the approach of putting class comments, data member documentation, and class usage in the header, and documentation of how the methods/functions work in the source files where they are defined. This has the benefit of not cluttering the header files. There certainly is some precedence for this in online discussions.

2. make_examples.sh:

   i. will only work with a g++ compiler in the user’s path.
   ii. Is referred to as build_examples.sh in the README.md file
   iii. is redundant with the cmake build system and isn’t portable. It should probably be removed.

   The `make_examples.sh` file has been removed and examples are built with CMake. This script was originally included for reference.

3. It appears that there are no tests associated with the library. This is a bit surprising - I would expect regression test coverage on the basic API functionality.

   The API is pretty simple and consists of two functions. Extensive examples are provided, which are compared to LBL data, and which, as published here, are identical to the results of the published radiation models. That said, a branch of the code is being developed that includes tests.

4. CMake build system:

   i. Consider installing a "RadLib.cmake" file for downstream usage by CMake-based projects. This helps downstream build systems configure for RadLib usage (setting include paths, etc.).

      This is a good point. The installation now includes `radlib.cmake` files, located by default in the `installed/cmake/` directory, for downstream usage.

   ii. probably shouldn't specify optimize or debug flags directly, as CMake will provide appropriate values on most platforms.

      The CMake build has been updated to reflect this.

   iii. the default build type isn't defaulting to Release for me; it remains blank.

      This appears to be working in the revised version of the code. Testing shows the value of CMAKE_BUILD_TYPE as set to Release if not otherwise set. This is specified at the very top of the base CMakeLists.txt file. Note that the build type can be overridden by IDE build settings, among other things, and that this may be a system issue specific to the reviewer.

   iv. I suggest not using verbose makefiles by default.

      The build has be updated so that verbose makefiles are no longer the default.

   v. Using GLOB to install the headers is not the appropriate CMake approach.

      The build updated accordingly; GLOB is no longer used to install header files.

   vi. the data files are not copied into the examples build directory, meaning that the example executables do not run.

      The original code has been updated and tested and this is now corrected.

   vii. The run-examples.sh script is not helpful as it is not installed into the build directory where the executables are produced and doesn't have path information to actually run the executables.

Executables for the examples are installed within the example folders (in addition to the build directories), so `run_examples.sh` runs without any issues.

viii. Using "doxygen" as a target is not ideal since it conflicts with the "doxygen" executable name. It still works fine though…

Build target name has been changed from "doxygen" to "docs" for safety. Note that building the documentation is off by default.

5. It appears that line-by-line data from HITEMP/HITRAN files cannot be loaded into RadLib. That's an unfortunate limitation, but not a deal-breaker.

   This is true. The code is not presently set up to load HITEMP/HITRAN data. This is a good suggestion and we would like to extend the model to allow LBL simulations in the future.

6. It looks like the software hard-codes Plank mean absorption coefficients as (fourth-order?) polynomial fits? Same for WSGG. There is no discussion of why this was chosen, how the coefficients were determined, or a characterization of its accuracy. Do you observe any problematic behavior with the fourth order polynomials over temperatures from 300 to 3000 K? Are these interpolants or regression of data?

   The software implements the PM and WSGG models as provided in the cited references, which use polynomial fits. Model details are noted in the cited references. Use of a polynomial fit is standard for WSGG models, and a polynomial fit to temperature for species for the PM model seems reasonable. The PM model used is the one advocated by the TNF workshop cited in the paper, which is standard in the combustion community. The temperature range is 300-2500 K for the PM model. This is now stated in the paper, and the code enforces this range. The range for the WSGG model is 300-2400 K. The range for the RCSLW model is 300-3000 K. Temperatures outside these bounds use these bounds for the WSGG and RCSLW models. This is now stated in the paper.

7. The two previous items combined lead to a significant limitation of RadLib: one cannot easily add new species or modify existing data that is used to generate the absorption coefficients since there has been internal preprocessing of (an unknown subset of) the HITEMP/HITRAN databases to produce curve fits. And given that this process is opaque, it isn't reproducible.

   The implemented models described in the cited literature. The novelty of the presented library is not the development of the absorption models, but the implementation, validation, and documentation of a library for application. Using RadLib to generate correlations for species using HITEMP/HITRAN is outside of the intended scope. We acknowledge that extra work is required to extend the models to additional species, or to extend the temperature ranges. However, the species included cover a very wide range of practical applications, certainly in the combustion field, and models for other species (e.g., for WSGG, and RCSLW) are often not available. Indeed, Bordbar's WSGG model is one of the few (if not the only one) that is provided for arbitrary compositions of CO2

and H2O, with others assuming fixed or limited ratios. That said, radlib is documented and while the code does not provide extension machinery directly, extending to additional species by following the existing code structure would not be difficult if such data/correlations were available.

8. RadLib only considers CO2 and H2O for WSGG, which is fairly limited. Even for Plank mean, only H2O, CO2, CO and CH4 are considered. NO and OH would be nice to include. It appears that including additional species would be a non-trivial undertaking.

   See our reply to the previous comment regarding additional species. For heat transfer applications in combustion, NO and OH are minor species and will not contribute in any meaningful way. CO2, H2O, and soot will drive the radiation in practical configurations. It would be nice to include CO in the WSGG model, and we would like to do this following Bordbar's approach. But even CO is a minor species compared to CO2, both in terms of its concentration in practical systems (usually), and its absorption coefficient on an equal concentration basis. CH4 was only included in the PM model from the TNF workshop since many of the fuels used there include CH4. But CH4 will largely be present at relatively low temperatures, not the highly radiating flame zones.

   We note that major revisions have been made to the paper text to clarify points like these for readers who do not specialize in, e.g., combustion processes or modeling and provide additional information about why these models were chosen for implementation in RadLib.

9. Documentation:

   i. Generating the documentation directly via doxygen v. 1.8.20 gives numerous warnings about obsolete tags and then fails because it is looking for a relative path "…/…/docs/doxygen" that doesn't exist. This should be fixed.
   ii. Generating the doxygen documentation via the build system target ("make doxygen") does seem to work fine.

   The build process has been updated so that documentation can be generated by the system target or manually by running the command `doxygen` in the docs folder. We have removed obsolete flags, and also updated the source documentation to be consistent with function signatures.

Reviewer 2

A radiation spectral property library is developed in this study using C++. A Planck-mean absorption coefficient-based model, a WSGG model and a RCSLM model from the literature are implemented in the package. Verification results are presented and discussed. Although the authors addressed an important issue of radiation modeling, the contribution is marginal in the reviewer's opinion. No new models/methods are proposed in this study. As the authors correctly pointed out, the solver for radiative transfer equation is equally important, which is not included

in the library. The coupling of a spectral model to a specific RTE solver, can have different levels of challenges depending on the combination. The design of the library doesn't really address any of the RTE-related issues, nor provide any new solutions to simplify the coupling of spectral models to RTEs. If the authors can demonstrate that the library can be coupled with popular CFD software and popular RTE solvers such as P1 and DOM, it would further improve the quality of this study. A few other concerns are listed as follows:

The authors thank the reviewer for their comments and suggestions. It is true that the library presented does not develop new models, but implementing and providing those models is nontrivial, and we believe makes a good contribution that is within the scope of this software journal.

We agree the reviewer's suggestion regarding coupling with popular CFD software and a corresponding RTE solver, and that this would strengthen the paper. We have made significant revisions to the paper and code in this regard. First, we developed a new Fortran interface that calls the underlying C++ code. Second, we coupled the code to the Fire Dynamics Simulator (FDS) code, developed by NIST. FDS is a Fortran code that required the new Fortran interface. FDS has several radiation models available including WSGG DOM implementation. Radlib was interfaced to this model by using the radlib Fortran module in the source code. We then replaced the existing calls to the functions for computing the absorption coefficient and weighting factors with calls to radlib. FDS does an outer loop over the gases/bands with inner loops over the local grid points. RadLib was not set up for this, since it computes the properties for all bands at a given point. Hence, direct use of RadLib would have been inefficient. As a result, we implemented a new interface function get_k_a_oneband, that facilitated implementation in FDS. In the revised paper, we present results comparing the WSGG and RCSLW models in FDS applied to the FM Burner validation case that is detailed in the FDS Validation Documentation. We hope that this effort will satisfy the reviewer and improve the paper as desired.

1. RADCAL data were used to generate the Planck Mean absorption coefficient. Based on the reviewer's experience, the Planck Mean absorption coefficients can have meaningful differences when generated from RADCAL and from HiTEMP2010. It is recommended a more recent database being used for the library.

   The Planck Mean absorption coefficients model as implemented in RadLib refers specifically to the radiation model in [3,5], which is one of the most common radiation models applied to turbulent combustion simulations. It was chosen because of its popularity and widespread use in combustion simulations (despite its limitations). That said, there is value in using the most current tools. Given the reviewer's experience with variance in the Planck Mean absorption coefficients as calculated from various databases, the authors will strongly consider adding an updated Planck Mean model using the most current available data. That said, the PM model implemented is generally applied in optically-thin situations with relatively low radiative transfer in which case the errors are not as significant.

2. Page 10, missing information on [INSERT RUNTIME COMPARISONS HERE].

   This has been corrected.

3. In Figure 2, the RCSLM seems to consistently perform better than WSGG, except in Example S2. In addition, WSGG performs worse than PM in Example S4. Can the authors explain why?

   The WSGG model coefficients presented were those from Bordbar's paper. These have since been updated and included in the revised code and we have likewise updated the simulation results in the paper. For the new results, the WSGG model no longer performs poorly for example S4. For example S2, the RCSLW model converges to the LBL results as the number of gases increases, but the WSGG model outperforms the RCSLW model for 4 gray gases. It is not clear why the WSGG model outperforms the RCSLW model for this case. We have added some relevant discussion to the paper. We do note that the WSGG model is empirical and contains very little representative physics, which makes it difficult to explain the behavior of the model.

4. Equation 6 appears to be inaccurate.

   Upon review, the authors find no errors in Equation 6, which matches Equation 20.65 of the general band model (of which the WSGG model is a subset) derivation in [2] and appears to be consistent with the other equations in the paper. The equation is q = int(I(s)sdΩ). The notation here is that I is a function of direction, but is itself a scalar so that I(s)s is equivalent to a vector I in direction s.

5. Typo: page 4, line 49, "relating them" -> "relating the"

   This phrase has been removed in the revision.

Reviewer 3

The Computer Program in Physics (CPiP) submission titled, "RadLib: a radiative heat transfer model library for CFD" by Stephens et al reports a library of radiative property models that is modular and can be interfaced with other radiation model components. The manuscript is well-written and well-organized. The works cited are reasonable. RadLib contains a gray Planck-mean (PM) model, a weighted sum of gray gases (WSGG) model, and the rank-correlated SLW model. This is definitely an important tool for the combustion community, where the radiation modeling is often oversimplified mainly because of the lack of readily available appropriate radiation model libraries! I am not aware of any open-source libraries that combine the three property models presented here. The models included in RadLib are already well-established and well-validated in the radiation community. The library is written in C++ and is supposed to work in any Linux-like system. The code is well commented, although the associated documentation needs to be improved (see major comment #1).

Considering all these, I think that this CPiP submission is definitely within the scope of the journal and of interest to the research community. However, the following concerns must be addressed before the submission is considered for publication.

The authors thank the reviewer for their insightful comments and suggestions. As members of the combustion community, we heartily agree that a tool like RadLib could benefit researchers and facilitate radiation model development for combustion CFD.

1. I could not successfully build and run the library in two different Linux systems. In both cases, first, the cmake returned an error: "CMake Error at c++/CMakeLists.txt:34 (install): install TARGETS given no ARCHIVE DESTINATION for static library target "radlib"." I could resolve this by adding ARCHIVE DESTINATION line on the c++/CMakeLists.txt file. But, then on during "make" my installation was interrupted several times because of missing packages in my Python installation. I would strongly recommend that the authors modify the installation instructions to include: a) list of dependencies (i.e., what compilers, what versions of python, what python packages, etc.), b) how to install the dependencies before building RadLib, c) a way to build RadLib with either only C++ or only Python. These installation notes do not necessarily need to be in the main manuscript, but they must be in the installation README of the code package.

   The CMake build system has been updated such that `ARCHIVE DESTINATION` is explicitly specified, so that error should no longer occur. A build option has been added that makes the Python interface installation optional. Note that the C++ source code is required to install the Python interface, so there is no option to build only the Python interface. This information has been added to the `README.md` files located in the root directory and the `build` directory along with a more thorough list of software dependencies and required Python packages. We have also done full tests of the installation and running of all examples on a desktop Mac, and a desktop Linux machine. The c++ and Fortran interfaces were tested on a large Linux-based cluster. The code also runs on a code ocean module.

2. The library includes PM, one WSGG, and a RCSLW model. The authors should clearly indicate the rationale of these choices (i.e., why only these three models) early on in the manuscript. Since this is intended for researchers who, presumably, are not experts in radiation modeling, the inclusion of these three models can be misleading. One might think that these three models are the most appropriate models for their simulations.

   Section 2 has been heavily revised and should better address this issue. In particular, at the beginning of section 2, we note the why these models were chosen. The three models are practically relevant, and represent a variation in complexity and accuracy.

3. RadLib is intended to be expanded with new radiation property models in the future and interfaced with a user-supplied solver module for RTE. A brief discussion on how to interface such an external solver module should be presented. There is an example of a ray-tracing solver presented in the code files, but a brief discussion on coupling one's own RTE solver is important in the manuscript. Additionally, a brief discussion on how a user can add a new radiative property model should also be included.

   Section 3 has been revised and extended to include more information on how users can include and interact with the RadLib library, including explicit references to example files that further illustrate usage of the library. We have also added a subsection to the

results discussion that describes the integration of RadLib with the Fire Dynamics Simulator (FDS) code developed by NIST. Adding additional radiative property models to RadLib would require creating another class object for the implementation. The intention would be for the new model to inherit from the `rad` base class and reimplement the interface functions `get_k_a` and `get_k_a_oneband`. Depending on the model, additional functionality may be needed. The Fortran and Python interfaces are wrapper functions that can be extended by paralleling the existing code, which is much simpler than writing these interfaces from scratch. A discussion on these points has been added to Section 3.

4. The Planck-mean absorption coefficient included in RadLib is based on TNF workshop data (from 2003). According to the references cited, these are fairly old correlations. If the authors use these data, I am concerned that the model parameters and correlations used in RadLib for the PM model may be obsolete and inaccurate. Can the authors please comment on this?

   We purposely chose the TNF workshop data for calculating Planck Mean absorption coefficients because it is one of the most common and widely used radiation models applied to turbulent combustion simulations, despite its age and limitations. Section 2.1 has been revised to include a more explicit discussion of why the TNF radiation model was chosen. Sections 4 and 5 include example cases and results that demonstrate the deficiencies of the PM model compared to the other models included, and some additional discussion is given there. We intend to extend the model to include updated PM data.

5. On page 13, the authors present a paragraph describing Figs. 2 and 3 - the comparison of various radiation property models present in RadLib in one-dimensional configurations. The comparisons are presented simply as observations without any explanation or reasoning why the models behave the way as seen in Fig. 2 and 3. If I understand correctly, the focus of the work presented here is not the comparison of the accuracy of the three models but to showcase the library. Therefore, these comparisons - specifically without any explanation of the results - may not be essential to the current manuscript, and can be shortened. These results do serve as descriptions of example cases provided in RadLib. On the same page, the authors say that "While ommitted [should be omitted] here for brevity, the implemented WSGG and RCSLW models give essentially identical results to those presented in [11, 14] such that these examples also serve as a validation of the implementation of the models." The authors should avoid qualitative description such as "essentially identical" in the context of validation and present a quantitative (e.g., % error) metric wherever possible. A strong validation is important for programs like this.

   While it is true that the purpose of this paper is to present the RadLib library rather than evaluate or compare the models, the authors believe that example case results in Figures 2 and 3 are important. These illustrated examples RadLib's capabilities, demonstrate the example cases provided with the code, and provide comparison between the models and with reference to the LBL data. Comparison between the models has relevance to the reviewer's second comment above regarding the rationale of the models chosen, and our

discussion of them in reply in the text. The reviewer's point about presentation without explanation is valid. The discussion in Section 5 has been expanded. Some of the results and discussion have changed since are now using updated parameters for the WSGG model that improves the agreement of that model, especially for Example S4. This makes the models for the different cases presented more consistent, lessening some of the burden for explaining anomalous behavior, though, due to the empirical nature of the PM and WSGG models, full explanations can still be difficult.

Regarding validation, we agree with the reviewer in being careful about the language used. We are fully confident in the implementations of the models presented. Model parameters were checked and rechecked, and results from RadLib were carefully compared to the corresponding model results presenting in the original papers. In the case of the RCSLW model, which is the most complex to implement, we had the benefit of discussions with the inventors of the model (noted in the Acknowledgements), and even compared our code output to their Fortran implementation. We have modified the text to avoid qualitative description.

6. The computational cost tables for two cases show a significantly different trend, which the authors attribute to "additional overhead required in performing the calculations." Can the authors be more specific as to what these overheads may be? They say that they have neglected the initialization and input/output costs. Also, do these CPU times presented include the cost for the ray-tracing solver as well? Are the grids kept the same for all configurations?

   We have modified the discussion slightly by moving the note about the cost not including model initialization and input/output earlier to make it clear that that applied to all results. Two cost comparisons are given: (1) cost of the property evaluation itself; and (2) cost of the full RTE solve (including the ray-tracing solution and property evaluation). Item (2) is relevant since property evaluations are not normally done in isolation, but part of a larger RTE solve, so that differences in the property model costs have less impact on the overall cost. This is now noted in the paper. The revision should be clear about the costs including the ray-tracing solver and the constant grids. Regarding the "overhead," the revision reorders the discussion and that word is not used. This discussion parallels what is noted here, that differences in the overall costs are smaller when accounting for the cost of the RTE solver as well as the property evaluation. (Note that Section 4.1 has since been moved to Section 5. It and the appropriate figure captions have also been revised for clearer communication of the points above.)

7. In line 53 on page 4, the authors claim to have CH4 property in RadLib but none of the validation cases contain CH4. Furthermore, for RCSLW, the refer to Pearson's work as a source for data of CO2, H2O, and CO without indicating the source data for CH4.

   CH4 is present only in the PM model sourced from the TNF Workshop [3,5], which includes CH4 absorption coefficients because most of the TNF Workshop target flames are fueled by CH4. In general, CH4 is not a significant radiatively participating species in combustion systems, but it is included in the PM model for completeness with the PM source. The revision notes differences in the models and species, and default values are

included for species in the interfaces (also now noted) so that users don't have to specify mole fractions for species that are not used in a given model.

MINOR:

1. It should be clarified that RadLib only provides radiation properties for non-scattering media.

   This clarification has been made explicitly in Section 2 and now appears elsewhere the text where appropriate.

2. In the program summary the description of the nature of the program is somewhat confusing from a grammatical construction standpoint. Particularly, the following part, "This presents a problem for practitioners who wish to use/implement radiation models for which [refers to what?] such models consitute [constitute?] only a small but important part of a larger simulation. Turbulent combustion simulations are one such example [example of what?]. Often, rudimentary assumptions [in what?] are made and this can negatively impact results."

   The program summary has been rewritten for clarity.

3. In Page 2, "In some cases, radiative gains or losses are small compared to other energy sources or heat transfer modes and radiation can be safely neglected, … difficult to simulate accurately without a robust radiation model." Please provide some references to support these arguments.

   This statement has been removed in the revision. In the spirit of this comment, we have added references to the text where needed to bolster weakly supported arguments. In particular, due to unrelated revisions, such discussion appears in Section 2.1 since it is most closely related to the Planck Mean model and its limitations.

4. Please explain all the symbols used in equations. For example, eta in Eqn. 1 (and subsequent equations), Eb in Eqn. 11.

   Text surrounding equations has been revised throughout to ensure explicit definitions of variables.

5. Page, 4: "Global models are an important class of radiation property models that make use of spectrally-integrated radiation properties and are usually versions of the weighted sum of gray gases (WSGG) model [1, 2]." This sentence is somewhat misleading. It may be more appropriate to think of WSGG models as special cases of SLW or FSK models.

   The authors agree that this statement could be potentially misleading. The second half of the sentence (beginning with ". . .and are usually. . .") has been removed.

6. In lines 48-52 on Page 4, the authors say that the absorption coefficients are calculated using some correlations after some curve-fitting to spectroscopic databases. I am not sure

what the authors refer to as correlations. There may be some correlations involved in WSGG models, but it is not clear to me where are correlations involved in RCSLW.

The absorption coefficients for the gray gases are developed from high resolution databased, and correlated, for each gray gas considered, as functions of the local gas state (temperature, pressure, and composition). The PM model uses a temperature correlation for each species absorption coefficient, with the overall absorption coefficient computed by combining the species. The WSGG model uses correlations developed for the gray gases based on emissivity calculations from the high-resolution databases, and treats the composition through the molar H2O/CO2 ratio. The RCSLW model's key tool is the absorption line blackbody distribution function (ALBDF), which is calculated using spectral data available from databases like HITEMP. See Solvjov 2017 (cited in the paper) for details. The revision includes such discussions for the individual models. The modification of the original statement is in the last paragraph in Section 2 before section 2.1.

7. On page 7, the authors mention that the PM model can be "reasonably accurate" in some cases and go on to say that, "The Planck Mean model is most appropriate under optically thin conditions with relatively low radiative transfer relative to other heat sources such as reactive heat release rates." The Planck Mean model will be appropriate in optically thin cases as there is very little reabsorption. This may or may not be connected with "relatively low radiative transfer relative to other heat sources." In fact, if the radiative heat transfer is much lower than chemical heat release, neglecting radiation altogether may also be reasonable! Although, the definition of "relatively low" is subjective.

   This discussion is modified in the revision. The PM model is not directly connected to optical thickness of flames. In combustion applications, the PM model is often used in situations that are optically thin. In such cases, the radiative losses are relatively low (often around 5% for laboratory jet flames), and use of the PM model may provide sufficient accuracy given that errors are active at the 5% level of the overall radiative losses, so not severe. When coupled with the optically thin assumption for RTE treatment, the radiative solve is relatively simple and inexpensive.

8. On the same page, lines 40-41, "This version of the WSGG model is advantageous because it allows for arbitrary CO2 and H2O compositions, increasing its accuracy and flexibility." Can the authors provide some references that show the increased accuracy and/or flexibility of this WSGG over any other WSGG?

   Two references for the chosen WSGG model are given earlier in the paragraph. The second (Bordbar et al. 2020) includes detailed comparisons between this model, its immediate predecessor (see Bordbar et al. 2014), five other WSGG models, and line-by-line calculations for four different test cases that show high accuracy over a wide range of molar ratio values. We have noted this in the revision. While other models may have performed better in individual tests, this model demonstrated consistent accuracy over a range of scenarios. For clarity, this reference has been added to the end of the aforementioned sentence so as to better indicate where to obtain relevant information.

9. With respect to Eqn 8, Mr is defined as molar ratio y_H2O/y_CO2. Are the authors using y as a symbol for mole fraction rather than mass fraction as is conventionally done?

   We have changed the notation in the paper to use x instead of y. This is consistent with our use in the code, and we also prefer x for mole fraction and y for mass fraction. Solovjov (RCSLW) and Bordbar (WSGG) both use Y for mole fraction though.

10. Please remove the words "[INSERT RUNTIME COMPARISONS HERE]" on Page 10.

    Done.

11. In lines 29-30 on page 13, please insert the units for Q in -80 and 200.

    Done.

12. In the Discussion (page 16), the authors write, "Neglecting radiation or using simple models like the optically thin assumption is adequate for some cases with simple geometry or limited chemical reactions…" This can be misleading. I am not sure if either the simple geometry or the limited chemical reactions give any indication of the importance of radiation. Rather, something like a radiant fraction or optical thickness may be a more appropriate metric to justify neglecting radiation or using an optically thin model.

    This is a good point. The revision should correct this. We partially answer this in reply to your comment above regarding page 7 that the "PM model can be 'reasonably accurate'". In particular, we are revising the discussion around the PM model to note that it is not an overly accurate model in comparison to the others, but it is widely used, and its use is warranted in situations with relatively low radiative losses that may occur, for example, in cases where radiative losses are low compared to heat release rates, or where flow timescales are low compared to radiative transfer timescales.

RadLib: a radiative property model library for CFD

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Abstract

RadLib is a C++ library of radiation property models that can be applied to variety of systems involving radiative heat transfer, including CFD simulations. RadLib includes three major radiation property models—Planck Mean (PM) absorption coefficients, the weighted sum of gray gases (WSGG) model, and the rank-correlation spectral line weighted-sum-of-gray-gases (RCSLW) model. RadLib includes C++, Python, and Fortran interfaces and can be expanded to include additional models.Several example cases illustrate the use of the models with an included ray-tracing solver and compare them in terms of accuracy relative to line-by-line solutions. A CFD example is provided of an ethylene burner in a compartment using Fire Dynamics Simulator (FDS). The computational cost of the models is compared. RadLib provides researchers with convenient access to validated radiation property models and a framework for further development.

Key words: radiative heat transfer, reacting flows, CFD, WSGG, RCSLW

PROGRAM SUMMARY

Program Title: RadLib
CPC Library link to program files: (to be added by Technical Editor)
Developer's repository link: https://github.com/BYUignite/radlib
Code Ocean capsule: https://codeocean.com/capsule/0997975/tree
Licensing provisions(please choose one): MIT
Programming language: C++, Fortran, Python
Nature of problem(approx. 50-250 words):
Radiative heat transfer in combustion CFD problems is typically neglected or over-

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simplified, resulting in significant error and inaccuracy in combustion simulations. Radiation modeling, however, often requires a high degree of specialization due to its complexity and the challenges associated with implementation in existing CFD codes, which presents a substantial obstacle to researchers who wish to address the inaccuracies introduced by insufficient radiative heat transfer modeling in combustion simulations.

Solution method(approx. 50-250 words):

We present RadLib, an open-source C++ library of validated radiation property models that can be applied alongside various RTE solution methods to ease some of the obstacles associated with radiation modeling for combustion CFD. The package includes C++, Fortran, and Python interfaces, several illustrative examples with a provided ray-tracing solver, and possibility for expansion to include additional radiation property models and interfaces.

Additional comments including restrictions and unusual features (approx. 50-250 words):

The library is intended to be used in Linux-like terminal applications.

1. Introduction

Modeling radiative heat transfer in participating media in high temperature systems is a challenging problem. Combustion is one of the key radiative transfer applications, and combustion CFD is uniquely challenging because it involves numerous tightly coupled physical phenomena—including multicomponent mass transfer, convective and radiative heat transfer, turbulent fluid dynamics, multi-phase and particle flows, and complex chemical reaction kinetics—that span many orders of magnitude in both length and time scales. Combustion simulations are often complicated by a lack of accurate radiation modeling, which can be difficult to implement and computationally expensive relative to overall simulation cost. Frequently, radiative heat transfer modeling in combustion systems is either neglected or oversimplified, resulting in significant errors flame temperatures [1]. Additionally, some late-stage flame phenomena, particularly soot behavior and flamesheet breakthrough, increasingly depend on and influence the magnitude of radiative heat losses and are difficult to simulate accurately without robust radiation modeling [2]. These problems motivated development of the RadLib library, which implements three radiation property models, with C++, Python, and Fortran interfaces, and provides a framework for additional models and further development, giving researchers convenient access to advanced radiation property

modeling tools.

The core mechanisms of radiative phenomena are physically and mathematically complex. Unlike other modes of heat transfer, radiation is governed by a set of integro-differential equations that depend on both direction and wavelength, known as the radiative transfer equations (RTE). Computational radiation solvers require two distinct but interconnected parts: (1) a solution approach for the radiative transfer equations (RTE) and (2) a radiative property model. Complexity, implementation, and computational costs of these two parts can vary widely, depending on the models chosen. The optically thin model for solution of the RTE is trivial, while the discrete ordinates model (DOM) and Reverse Monte Carlo Ray Tracing (RMCRC) model, among others, are significantly more involved. Similarly for radiation property models, which range from simple correlations for mean absorption coefficients, to gray gas models such as the weighted sum of gray gas model (WSGG), to the more advanced Spectral Line WSGG (SLW) family of model, to full line-by-line (LBL) treatment. In practical engineering simulations, the solution of the RTE is often the most complex and costly part of radiative simulation, but advanced property models, such as the Rank Correlated SLW (RCSLW), discussed here, are nontrivial models to understand, implement, and validate. RadLib addresses this second radiative property model part of radiation simulation by providing a set of implemented and validated radiation property models that can be applied to various solution approaches for the RTE.

For an absorbing, emitting, and non-scattering medium (considered here), the RTE for intensity I at a specified wavenumber η in unit direction $\mathbf{s}$ is described by

$$\frac{dI_\eta}{ds} = -\kappa_\eta I_\eta + \kappa_\eta I_{b,\eta}, \tag{1}$$

where I_η is the radiative spectral intensity, $I_{b,\eta}$ is the spectral blackbody radiative intensity (or Planck function), κ_η is the spectral absorption coefficient of the medium, and s is a path length along direction $\mathbf{s}$. Solving the RTE requires information about the radiative properties of the materials and media in the system. Radiative property data typically takes the form of radiation absorption coefficients κ, which are provided by a radiation property model. Gas absorption spectra consist of millions of spectral lines corresponding to the individual quantum mechanical energy levels of gas molecules, and depends on the local thermochemical state of the system (e.g., temperature, pressure, and composition). Radiation property models, including those im-

plemented in RadLib, are typically developed using high-resolution spectral databases like HITRAN and HITEMP [3] in order to calculate spectral absorption coefficients, thus reducing or simplifying the huge amount of spectral data by using correlations and modeling assumptions [4].

The direct solution of the spectral RTE using so-called line-by-line calculations in which the RTE is solved for each individual spectral line is computationally prohibitive for most practical configurations and is used primarily for model validation. Some band models rely on estimated or averaged "line-of-sight" property values that cannot be directly incorporated into the RTE. Modern band models require high-resolution databases and reorder emission levels rather than averaging across sequential absorption bands, but these cant lose accuracy when applied to nonhomogeneous media and may still require large numbers of RTE evaluations [1].

Global models are an important class of radiation property models that use spectrally-integrated radiation properties [1, 2, 5]. Assuming spectrally uniform (gray) properties over a wavenumber region j, we can integrate Eq. 1 over the fixed wavenumber ranges η_j to obtain

$$\frac{dI_j}{ds} = -\kappa_j I_j + a_j \kappa_j I_b, \qquad j = 0, 1, ..., n, \tag{2}$$

where I_b is the blackbody intensity, I_j is the radiative intensity in the region defined by gray gas j, κ_j is the spectrally integrated absorption coefficient for gray gas j, and a_j is a weighting factor defined by

$$a_j = \frac{\int_{\eta_j} I_{b,\eta} d\eta}{I_b}, \tag{3}$$

$$\sum_j a_j = 1. \tag{4}$$

Given spatial profiles of κ_j and a_j, Eq. 2 can be evaluated for each of the n gray gases. Normally, an additional "clear gas", $j = 0$, is included that represents transparent windows in the spectrum for which $\kappa_0 = 0$. This gray gas approach allows calculation of the total radiative intensity I by summing the individual gray gas:

$$I = \int_{\eta=0}^{\infty} I_\eta d\eta = \sum_{j=1}^{n} I_j. \tag{5}$$

The heat flux $\mathbf{q}$ (in units of kW/m^2) and volumetric radiative heat source Q (kW/m^3) can be calculated by integrating over directional solid angles ($\mathbf{s}\Omega$) on the sphere and finding the divergence of the resulting vector field,

$$\mathbf{q} = \int_{4\pi} I(\mathbf{s})\mathbf{s} d\Omega. \tag{6}$$

$$Q = -\nabla \cdot \mathbf{q}. \tag{7}$$

Global models are especially attractive in computational heat transfer applications because they can provide good accuracy while limiting computational costs.

With RadLib, we aim to provide researchers with a convenient access point for radiative property models that can be interfaced with various RTE solution approaches suitable for CFD applications. RadLib is a C++ library with optional Python and Fortran interfaces. RadLib calculates radiation absorption coefficients and weighting factors for use in global radiation models. Expansion to other radiative properties and model types is possible. Three models are fully implemented and validated.

2. Model descriptions

At present, RadLib includes three radiation property models of varying complexity: Planck Mean absorption coefficients using the optically thin approximation, a weighted sum of gray gases (WSGG) model, and the rank-correlated spectral line weighted-sum-of-gray-gases (RCSLW) model. These models were chosen for their relevance to practical radiative heat transfer simulations. They represent increasing levels of complexity, computational cost, and accuracy. Each model is discussed in more detail in the following sections.

Radiation absorption coefficients are typically calculated via correlations developed from high-resolution spectral databases like RADCAL, HITRAN, and HITEMP [3, 6] that relate spectral line strength to properties such as temperature, pressure, and gas composition [4]. At present, RadLib considers up to four gas species (H_2O, CO, CO_2, and CH_4), depending on the model, and soot. The property models implemented in RadLib apply only to non-scattering media.

2.1. Planck Mean absorption coefficients

The Planck Mean (PM) model is the simplest of the three models implemented. This model assumes a single gray gas and computes the absorption coefficient as a function of temperature, pressure, and gas composition.

The particular version of the model implemented is from the Turbulent Nonpremixed Flames (TNF) workshop [7]. This is a long-running collaboration between experimental and computational researchers in turbulent combustion [8, 9]. The workshop includes a number of laboratory jet flames that have been extensively researched for flame temperature, velocity, and composition profiles, and these serve as target flames for computational scientists to validate simulations and models. The PM model implemented here is the one advocated (and hence widely used) by the TNF workshop.

For each species, the PM model provides the absorption coefficient as fourth or fifth order polynomial fits in one or two temperature ranges to $\kappa(T)$ values computed from the RADCAL database [6]. See [7] for details and references. The PM model here considers the species CO_2, H_2O, CO, CH_4. The last two species have lower absorption than the first two, but are included because CH_4 and syngas (consisting of CO and H_2) are common fuels in combustion applications and so are present in the TNF flames in high concentrations in the fuel stream. (CO is also a common species in rich flame regions and is also included in the RCSLW model.)

The PM model is not as accurate as the other two models considered, and this is illustrated in Section 5. It is implemented in RadLib primarily for comparison and evaluation against other radiation property models because of its relatively common use in some simulations. The model has been reported to overpredict radiative losses and underpredict flame temperature by as much as 100 K or more [10–12], though this will depend strongly on the geometric configuration. Accurate results have been reported for hydrogen jet flames [13].

The PM model is often used in conjunction with the optically-thin approximation for solving the RTE, in which case the radiative source term of the energy transport equation is particularly simple, and the overall computational cost of the radiative treatment is negligible in comparison to other aspects of a reacting flow simulation. Many smaller combustion applications are radiatively thin, and have smaller radiative heat loss. It is not uncommon for non-sooting laboratory-scale research jet flames to have radiative losses of around 5%. At these levels, the accuracy of the radiative property model is not as crucial, and simpler models like the PM model are appropriate.

2.2. Weighted sum of gray gases (WSGG)

Weighted sum of gray gases (WSGG) models generate radiation absorption coefficients for use with the spectrally integrated RTE (Eq. 2). RadLib implements the WSGG model presented by Bordbar et al. [14, 15]. This model computes emissivity for varying gas temperature, mixture composition, and path length using the HITEMP 2010 database [3]. The k_j and a_j are then correlated to these results using polynomial fits summarized below. The model considers mixtures of gaseous CO_2 and H_2O, the two most significant radiatively participating species in most combustion environments, using four gray gases and one clear gas. Absorption coefficients are calculated by

$$\kappa_j = \sum_{k=0}^{4} d_{j,k} M_r^k, \tag{8}$$

where κ_j is the absorption coefficient for gray gas j, $d_{j,k}$ is a correlated model coefficient, and M_r is the molar ratio $x_{\mathrm{H_2O}}/x_{\mathrm{CO_2}}$. The weight factors are calculated by

$$a_j = \sum_{k=0}^{4} b_{j,k} T_r^k, \tag{9}$$

where a_j is the weighting factor for gas j, $b_{i,j}$ is computed as shown below, and T_r is a scaled temperature equal to T/T_{ref} with T_{ref}=1200 K. The valid temperature range of the model is 300-2400 K; temperatures outside this range use the value at the respective bound. The value of $b_{i,j}$ is calculated by

$$b_{j,k} = \sum_{i=0}^{4} C_{j,k,i} M_r^i, \tag{10}$$

where $C_{j,k,i}$ is a correlated model coefficient. The model coefficients $d_{j,k}$ and $C_{j,k,i}$ are provided by Bordbar et al. [14, 15] but updated values are used in RadLib.

This particular WSGG model was chosen for RadLib for its performance, accuracy, and flexibility. Most WSGG models are limited to specific values of the molar H_2O–CO_2 ratio, or to a limited range of values. This is true of Bordbar et al.'s 2014 model [14], which used correlations valid for $0.01 \leq M_r \leq 4$. That paper summarizes a number of WSGG models and gives the applicable molar ratio range for several recent WSGG model versions. Bordbar et al. [15] extended the molar ratio range to arbitrary values

by interpolating κ_j and a_j between the pure component values and the corresponding limit on M_r for values outside of the correlated range, and that is the model implemented here.

2.3. Rank Correlated SLW (RCSLW)

The spectral line-weighted-sum-of-gray-gases (SLW) model represents a family of global approaches to radiative heat transfer in high-temperature gases that also includes the absorption distribution function (ADF) and full spectrum k-distribution (FSK) models, all of which are based on the same fundamental principle in modeling the gas absorption spectrum [16]. In order to extend their spectral models from isothermal, homogeneous composition gases to non-isothermal, non-homogeneous composition gases, these models use a reference approach in which radiative properties at local gas states are computed with respect to properties a at reference state. Such approaches, however, generally lack consistent reference states and can yield significant errors in cases with large spatial temperature gradients [17]. The Rank Correlated SLW (RCSLW) model is a unique extension of the generalized SLW model that does not require a specified gas reference state.

The RCSLW model was chosen for RadLib for its accuracy and performance compared to other SLW and WSGG modeling approaches. A recent comparison of SLW modeling approaches revealed that "the Rank Correlated SLW model is the most robust of all models, and demonstrates that it can achieve accurate solutions with as few as 3–5 gray gases" [18]. The literature indicates that the RCSLW model has not yet been applied to turbulent combustion simulations [1, 19]. We provide an example below using the Fire Dynamics Simulator (FDS) [20]. Other SLW models have been applied to gas–soot mixtures [21, 22] and high-temperature non-isothermal gases [23, 24] with results that suggest their good applicability to combustion systems.

RadLib implements the RCSLW method presented by Solovjov et al. [17] as method I.2.2, which gives the best and most consistent results of the SLW methods discussed in the aforementioned study. A summary of the general SLW method and the RCSLW method are presented here, but more detailed information about these and other SLW methods can be found in the literature [16, 17, 21, 23, 25–28].

SLW and WSGG models are similar in that they approximate real gas mixtures with a set of radiatively gray gases, but differ in the way the gray gases are constructed. In traditional WSGG models, the component gases are only conceptually gray, and the absorption coefficients and weights are

determined empirically [18]. In SLW approaches, however, the gases are gray in a given spectral band by construction. Rather than defining a gray gas j by integrating over a band of sequential wavenumbers η (which may have highly variable absorption coefficients), SLW models define a gray gas j by integrating over a set of nonsequential wavenumbers that correspond to a given band of the absorption cross section C_η with values constant to within the width of the band.

The absorption cross section is related to the absorption coefficient by $\kappa_\eta = C_\eta N$, where N is the molar density of the radiatively participating gas. Using Solovjov's notation in [17], $\Delta_j = \{\eta : \tilde{C}_{j-1} < C_\eta < \tilde{C}_j\}$ is defined as the set of wavenumbers that constitute the gray gas j, where $\tilde{C}$ denotes a cross section boundary between two gray gases. Hence, in SLW models, the gases in a given band are gray to within the width $\tilde{C}_j - \tilde{C}_{j-1}$.

The gray gas weight a_j is the fraction of blackbody emission from the set of wavenumbers Δ_j that correspond to a given cross-section band j. Weights are computed using the absorption line blackbody distribution function (ALBDF) [29], which gives the fraction of total blackbody emission from η corresponding to absorption cross sections smaller than an arbitrary absorption cross-section C:

$$F(C, \boldsymbol{\phi}, T) = \frac{1}{\sigma T^4} \int_{\{\eta: C_\eta(\eta, \boldsymbol{\phi}) < C\}} E_b(\eta, T) d\eta, \tag{11}$$

where ϕ represents the thermodynamic state, σ is the Stefan-Boltzmann constant, T is temperature, and $E_b(\eta, T)$ is the blackbody emission at a given wavenumber η and temperature T. As a result, a specific gray gas weight a_j can be calculated as the difference between the ALBDF values at its cross-section boundaries:

$$a_j = F(\tilde{C}_j, \boldsymbol{\phi}, T) - F(\tilde{C}_{j-1}, \boldsymbol{\phi}, T). \tag{12}$$

Note that F varies between zero and one and is monotonic in C, which permits calculation of an inverse ALBDF $C(F, \boldsymbol{\phi}, T)$.

For multicomponent gas mixtures, the mixture absorption cross section C_η is defined as a weighted sum of its component absorption cross sections [25]. The RCSLW implementation considers H_2O, CO_2, and CO, for which the mixture absorption cross section for a given gray gas is given by

$$C_\eta = x_{\mathrm{CO_2}} C_{\mathrm{CO_2},\eta} + x_{\mathrm{H_2O}} C_{\mathrm{H_2O},\eta} + x_{\mathrm{CO}} C_{\mathrm{CO},\eta}, \tag{13}$$

where x denotes mole fraction. Assuming that the absorption cross sections of each species are statistically independent, the mixture ALBDF for a given gray gas can be computed using the multiplication method [25]:

$$F_\eta(C_\eta) = F_{\mathrm{CO_2},\eta}\left(\frac{C_\eta}{x_{\mathrm{CO_2}}}\right) F_{\mathrm{H_2O},\eta}\left(\frac{C_\eta}{x_{\mathrm{H_2O}}}\right) F_{\mathrm{CO},\eta}\left(\frac{C_\eta}{x_{\mathrm{CO}}}\right). \tag{14}$$

Here, the $\boldsymbol{\phi}$ and T arguments of F are omitted from Eq. 14 for clarity.

The spectrally integrated RTE (Eq. 2) assumes the sets Δ_j are independent of spatial position $\mathbf{x}$, but C_η depends on the thermodynamic state (denoted by vector $\boldsymbol{\phi}$), which does vary spatially. Hence, a spatially-fixed Δ_j with spatially varying $\boldsymbol{\phi}$ implies a spatial variation in C_j and $\tilde{C}_j$. The RCSLW model uses the notion of rank correlation to handle this spatial variation in the ALBDF. Consider two positions with thermodynamic states $\boldsymbol{\phi}_1$ and $\boldsymbol{\phi}_2$ with corresponding absorption cross section spectra $C_\eta(\eta, \boldsymbol{\phi}_1)$, and $C_\eta(\eta, \boldsymbol{\phi}_2)$ and let $\hat{C}_1 \equiv C_\eta(\hat{\eta}, \boldsymbol{\phi}_1)$ and $\hat{C}_2 \equiv C_\eta(\hat{\eta}, \boldsymbol{\phi}_2)$ denote the cross sections at some wavenumber $\hat{\eta}$. For each spectrum, we define the set of wavenumbers that give cross sections less than $\hat{C}$ as

$$H_1 = \{\eta : C_\eta(\eta, \boldsymbol{\phi}_1) < \hat{C}_1\}, \tag{15}$$

$$H_2 = \{\eta : C_\eta(\eta, \boldsymbol{\phi}_2) < \hat{C}_2\}. \tag{16}$$

If $H_1 = H_2$ for an arbitrary $\hat{\eta}$, then the spectra $C_\eta(\eta, \boldsymbol{\phi}_1)$ and $C_\eta(\eta, \boldsymbol{\phi}_2)$ are said to be rank correlated.

The RCSLW model uses rank correlation as follows. Consider Eq. 11 evaluated at an arbitrary reference temperature T_r for thermodynamic states ϕ_1 and ϕ_2 as detailed above:

$$F(\hat{C}_1, \boldsymbol{\phi}_1, T_r) = \frac{1}{\sigma T_r^4} \int_{H_1} E_b(\eta, T_r) d\eta, \tag{17}$$

$$F(\hat{C}_2, \boldsymbol{\phi}_2, T_r) = \frac{1}{\sigma T_r^4} \int_{H_2} E_b(\eta, T_r) d\eta. \tag{18}$$

Since $C_\eta(\eta, \boldsymbol{\phi}_1)$ and $C_\eta(\eta, \boldsymbol{\phi}_2)$ are rank correlated (by definition), $H_1 = H_2$ and we have

$$F(\hat{C}_1, \boldsymbol{\phi}_1, T_r) = F(\hat{C}_2, \boldsymbol{\phi}_2, T_r). \tag{19}$$

Recall that the ALBDF can be inverted, so if $\hat{C}_1$ and $\boldsymbol{\phi}_1$ are known, we can compute $F = F(\hat{C}_1, \boldsymbol{\phi_1}, T_r)$ and then invert F to obtain $\hat{C}_2$ at $\boldsymbol{\phi}_2$. Note that

Eq. 19 holds for arbitrary states $\boldsymbol{\phi}_1$ and $\boldsymbol{\phi}_2$, so any known $F = F(C, \boldsymbol{\phi}, T)$ can be inverted to get C at the corresponding state $\boldsymbol{\phi}$.

Given the concepts summarized above, the RCSLW model is applied to a problem of interest to calculate radiation absorption coefficients and weights as follows:

1. Specify a reference temperature T_r as the average temperature on the domain of interest [21]. Note that this is not the same as specifying a reference state $\boldsymbol{\phi} = \boldsymbol{\phi}_r(T_r, x_r, P_r)$ as in done for SLW reference approaches.
2. Specify a collection of F_j points and $\tilde{F}_j$ boundary values such that F_j lies between $\tilde{F}_j$ and $\tilde{F}_{j-1}$. These apply to all spatial positions.
3. Invert the ALBDF to calculate C_j and $\tilde{C}_j$ at the corresponding thermodynamic state $\boldsymbol{\phi}$ and any spatial position where $C_j = C(F_j, \boldsymbol{\phi}, T_r)$ and $\tilde{C}_j = C(\tilde{F}_j, \boldsymbol{\phi}, T_r)$
4. Compute the gray gas absorption coefficients $\kappa_j = C_j N$.
5. Compute the gray gas weights $a_j = F(\tilde{C}_j, \boldsymbol{\phi}, T) - F(\tilde{C}_{j-1}, \boldsymbol{\phi}, T)$ (Eq. 12) with the C_j and $\tilde{C}_j$ values calculated in Step 3, the local thermodynamic state $\boldsymbol{\phi}$, and the local temperature T.

The ALBDF data for H_2O, CO_2, and CO—valid for pressures between 0.1 atm and 50 atm and temperatures between 300 K and 3000 K—are provided by Pearson et al. [29] and can be accessed in both correlated and tabulated form at [30]. Temperatures outside the stated range use the value at the respective bound. RadLib uses the tabulated data coupled with multilinear interpolation; both the tabulated data and the multilinear interpolator are included with the RadLib package as part of the RCSLW method.

2.4. Soot

Soot is accounted for in all three implemented models. Soot particles are assumed to be unagglomerated spheres that absorb and emit radiation at all wavelengths such that their optical properties can be determined using the Rayleigh small particle limit. This assumption implies that radiation scattering may be neglected because unagglomerated soot particles in the Rayleigh regime are still small relative to the wavelength of infrared radiation in flames [21, 31]. The spectral soot absorption coefficient is given by

$$\kappa_{s,\eta} = C_0 f_v \eta, \quad C_0 = \frac{36\pi n k}{(n^2 - k^2 + 2)^2 + 4n^2 k^2}, \tag{20}$$

where n and k are the real and imaginary parts of the soot complex index of refraction, respectively, and f_v is the soot volume fraction [2, 21]. Various values for the refraction index have been proposed and applied [32–38]. RadLib uses the values $n = 1.75$ and $k = 1.03$ [38], resulting in a value of $C_0 = 7.03$, which is nearly the same as the value of $C_0 = 7.0$ used by Solovjov and Webb [21] to study radiative transfer in sooty gas mixtures. The Planck mean and Rosseland mean soot absorption coefficients are given in [2] as $\kappa_s = 3.83 f_v C_0 T / C_2$ and $\kappa_s = 3.60 f_v C_0 T / C_2$, respectively. Due to the small difference between the coefficients in these two expressions, the mean value suggested by [2, 39] is used in RadLib's soot calculations:

$$\kappa_{soot} = 3.72 \frac{f_v C_0 T}{C_2}, \tag{21}$$

where T is the temperature and $C_2 = 0.014388$ m K is a Planck function constant [2].

In the Planck Mean model, which treats a gas mixture as one gray gas, the soot absorption coefficient calculated from Eq. 21 is simply added to the gas absorption coefficient. Using the given values of C_0 and C_2 above, the expression for the soot absorption coefficient simplifies to $\kappa_s = 1817 f_v T$ with units of m^{-1}.

In the WSGG model, the soot absorption coefficient is also computed using Eq. 21 but then added to each of the gray gases separately [40]. Because soot radiates across all wavelengths, its absorption coefficient is added to the value of the clear gas in addition to the values of the four gray gases. The gas weights a_j are not changed. This model yields the expected behavior in the soot-only and gas-only limits.

The WSGG soot treatment can be applied to the RCSLW model as well. Alternatively, the RCSLW model's formulation permits a spectral soot treatment in the same manner as the gas species [21]. Calculation of the soot ALBDF is facilitated by the simple η dependence of $\kappa_{s,\eta}$ in Eq. 20. The fraction of total blackbody emission at wavenumbers below η is computed directly using a series expansion presented by Chang and Rhee [41]. The soot ALBDF is then included in the product of species ALBDFs to obtain the mixture ALBDF, as in Eq. 14.

3. Software Description

RadLib is an object-oriented C++ library that includes C++, Python, and Fortran interfaces. Upon initial download, the RadLib package contains

four subdirectories:

- `src` contains the RadLib source code;
- `examples` contains instructive example cases, including a simple interface and solver for a parallel planes geometry;
- `data` contains ALBDF data tables required for the RCSLW model; and
- `docs` contains files used to optionally generate code documentation with Doxygen.

An additional directory, `installed`, is created and populated with RadLib's executables and header files during installation if no other installation location is specified. The `src` and `examples` directories are further divided into `c++`, `python`, and `fortran` subdirectories to differentiate between interfaces.

RadLib installation is automated with CMake as follows. Inside the downloaded `radlib` folder, the user creates and enters a `build` directory, then enters the commands `cmake ..`, followed by `make`, followed by `make install`. Project options are specified by editing the top-level `CMakeLists.txt` file where the options are clearly marked. These can also be specified at the command line. Options include specifying the system installation location, which defaults to `radlib/installed`; options to build the Python and Fortran interfaces; options to build examples for C++, Python, and Fortran; and an option to build the documentation. Included `Readme.md` files provide additional information.

The code installation folder includes directories `include` containing header files and a Fortran module file, `lib` containing library files for each interface, `cmake` with relocatable CMake files for downstream usage, and `rcslw_data` containing binary data files used by the RCSLW model. These binary files contain the ALBDF functions for a given species at a given pressure (in atm units), as indicated by the file name. The `include` directory contains the following interface header and module (Fortran) files:

- `rad_planck_mean.h`,
- `rad_wsgg.h`,
- `rad_rcslw.h`,
- `rad_module.mod`.

The C++ and Fortran libraries in the `lib` folder are

- `libradlib.a`,
- `libradlib_fortran.a`.

This folder also contains the Python module. If the Python interface is built, the location of the installed Python package needs to be added to the `PYTHONPATH` environment variable. A command to do this is provided at the end of the installation.

To use RadLib in C++, a user code includes the header file for the desired radiation model, e.g., `#include "rad_rcslw.h"`. For Fortran, a `use rad_module` statement provides access to the required interface functions. The Python interface functions are loaded from the `pyrad` module, as in `from pyrad import pyrad_rcslw`. Such usage is demonstrated in the code listing for the examples discussed below. Compilation of C++ and Fortran programs requires specification of the header/module and library directory locations and linking against the installed libraries (`libradlib.a` for C++ and both `libradlib.a` and `libradlib_fortran.a` for Fortran).

Figure 1 illustrates the basic structure of using RadLib in a generic one-dimensional RTE solution. The RadLib library generates absorption coefficients and their weighting factors for use within an appropriate RTE solver. A user first creates a radiation object, and then makes calls to one of two primary functions: `get_k_a()`, or `get_k_a_oneband()`. These two functions take the arguments for temperature (K), pressure (Pa), soot volume fraction, and mole fractions of H_2O, CO_2, CO, and CH_4. The WSGG model does not account for CO or CH_4, and only the PM model includes CH_4. A uniform interface is facilitated by giving default values of 0.0 for the CO and CH_4 mole fraction parameters so that these do not need to be specified for models that do not make use of them. The `get_k_a()` function computes a vector of absorption coefficients and a vector of weight factors, with elements corresponding to each clear and gray gas considered in the model (with the clear gas coming first). The PM model only considers one gas and the vectors are of unity size. The `get_k_a_oneband()` computes the absorption coefficient and weight factor (as scalar values) for a single gas (or *band*), whose index (starting at zero for all interfaces) is provided as an additional argument. This option to compute the properties for a single gas/band can be important for efficient implementation in some solvers, e.g., in the Fire Dynamics Simulation (FDS), discussed below [20]. The absorption coefficients

and weights are set through the function argument list for the C++ and Fortran interfaces, and as return values for the Python interface. Additional details are included in the program documentation and code listing.

The RadLib source code is build around a base class called `rad` from which the individual property models, e.g., `rad_rcslw`, inherit. To extend RadLib to include new radiative property models, a user would create a new derived class for the model that inherits from the `rad` base class. The interface functions `get_k_a` and `get_k_a_oneband` would be reimplemented in the new model. Additional functions and capabilities could be added as desired. The Fortran and Python interface codes consist of wrapper functions to the underlying C++. These can be easily extended by paralleling the existing interface functions.

4. Examples

The RadLib package includes several example cases that illustrate the behavior of the models and interfaces. The examples compare the PM, WSGG, and RCSLW models via output heat flux q or volumetric heat source Q in one-dimensional configurations with varying gas compositions and temperatures. The RTE is solved between two parallel plates with a ray-tracing code, included in the RadLib package. Results for each case are presented alongside the line-by-line (LBL) data from the respective references.

Table 1 summarizes the example cases. Each case is labeled according to its source—Solvojov et al. [17] (S), Bordbar et al. [15] (B), or Solovjov et al. [21] (Sb)—and the number of each example corresponds to the example number in its respective reference. Each example case consists of one or more gas layers ("slabs") bounded by black walls. Example S1 consists of two adjacent gas layers with identical species compositions: one hot layer of constant thickness and one cold layer of varying thickness. In Example S2, the two gas layers are isothermal but differ in the value of the CO_2 mole fraction, where the layer thickness of the "thin" slab (with the smaller CO_2 mole fraction) varies. Example S3 applies parabolic temperature and H_2O mole fraction profiles across a single gas layer. Example S4 divides the gas into three equally-spaced layers and applies a triangular temperature profile to the middle layer and a constant temperature to the two outer layers. Example S5 uses a half-sinusoid temperature profile that decreases from 1500 to 500 K applied to a single gas layer of constant composition. Example B3 has symmetric temperature and H_2O mole fraction profiles with central peaks

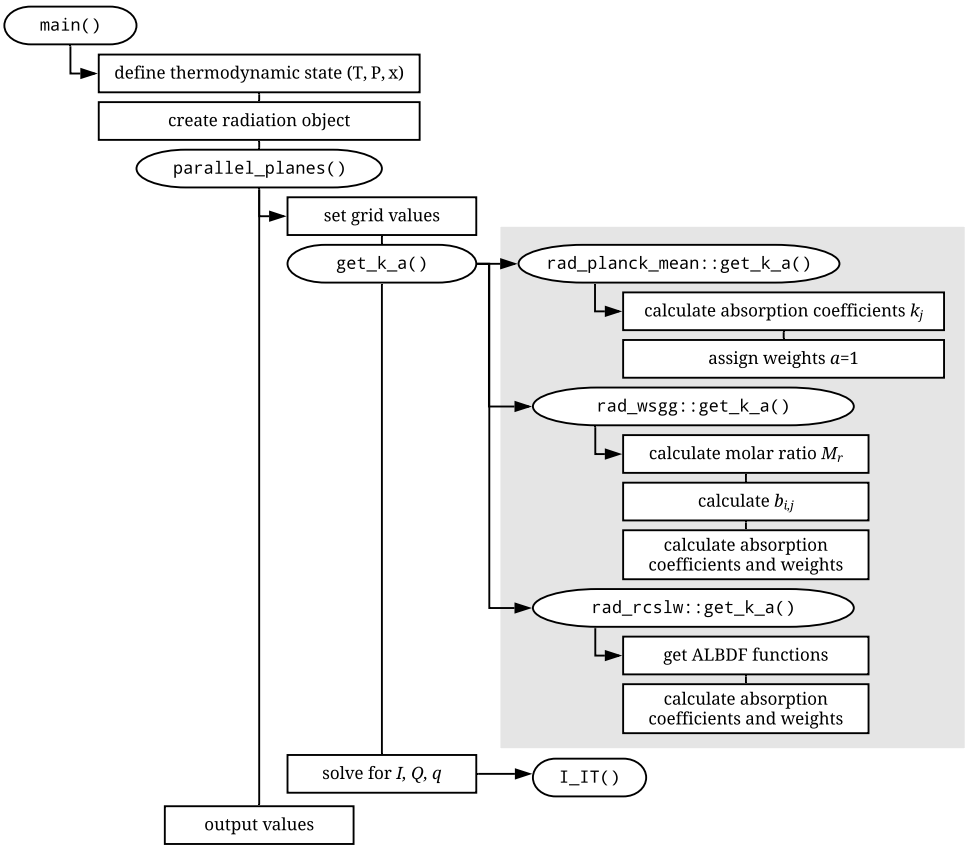

Figure 1: Example workflow diagram. Highlighted areas are part of the RadLib library; other areas represent example infrastructure for using the package.

Example	T(K)	x_{H2O} x_{CO2} (mole frac.)	L (m)	T_{walls} (K)	Ref.
S1	$T(x<0.5)=2000$; $T(x>0.5)=300$	$x_{CO2}=0.1$, $x_{H2O}=0.2$	0.5-2.5	cold, cold	[17]
S2	T=1000	$x_{CO2}(x<0.5)=0.4$, $x_{CO2}(x>0.5)=0.1$ $x_{H2O}=0.0$	0.5-2.5	cold, cold	[17]
S3	$T(x)=4000x(L-x)/L^2+800$	$x_{H2O}(x)=0.8x(L-x)/L^2+0.12$ $x_{CO2}=0$	1	800, 800	[17]
S4	middle third triangular to 2500	$x_{H2O}=0.1$, $x_{CO2}=0$	0.3	500, 500	[17]
S5	$T(x)=1000+500\cos(\pi x/L)$	$x_{H2O}=0.1$, $x_{CO2}=0$	2	1500, 500	[17]
B3	$T(x)=400+1400\sin(\pi x/L)^2$	$x_{H2O}(x)=0.0001+0.9999\sin(\pi x/L)^2$ $x_{CO2}=1-x_{H2O}$	1	400, 400	[15]
Sb1	$T=1000$	$x_{H2O}=0.2$, $x_{CO2}=0.1$, $x_{CO}=0.03$	1	cold, cold	[21]

Table 1: Summary of example cases. All cases use $P = 1$ atm and black walls.

of 1800 K and 1, respectively (with $x_{CO2} = 1 - x_{H2O}$). Example Sb1 consists of a single gas with a uniform temperature and composition profile and soot radiation.

The examples are provided with the RadLib code and implemented in both C++ and Python. A Juptyer notebook is provided with the Python examples that runs the examples, displays the plots, and saves the plots to PDF files. Python and Cython versions of the one-dimensional solver `parallel_planes.py` are provided for convenience.

These cases are intended to illustrate the use of the RadLib library and are not exhaustive. Details about these examples and their motivations can be found in their respective references. Comparison of these results to the LBL data, shown here, serve as model validation. For WSGG and RCSLW, direct comparison (not shown) of RadLib was made to examples presented in the model references with identical results (up to the resolution of the available data), which serves as verification of the implementation.

5. Results and Discussion

Figures 2 and 3 display comparative results for the PM, WSGG, and RCSLW models implemented by RadLib in the example case configurations summarized in Table 1. These plots are included to demonstrate the examples that are provided with the code, and to compare the models to give an indication of their relative accuracy. In all examples, the RCSLW model data is computed using four gray gases ($n = 4$) and one clear gas for consistent comparison to the WSGG model, with the exception of Example S5, in which the number of gray gases in the RCSLW model is varied. The RCSLW model is initialized using the mean temperature and composition on the domain for all cases except Example S5, which uses the maximum temperature.

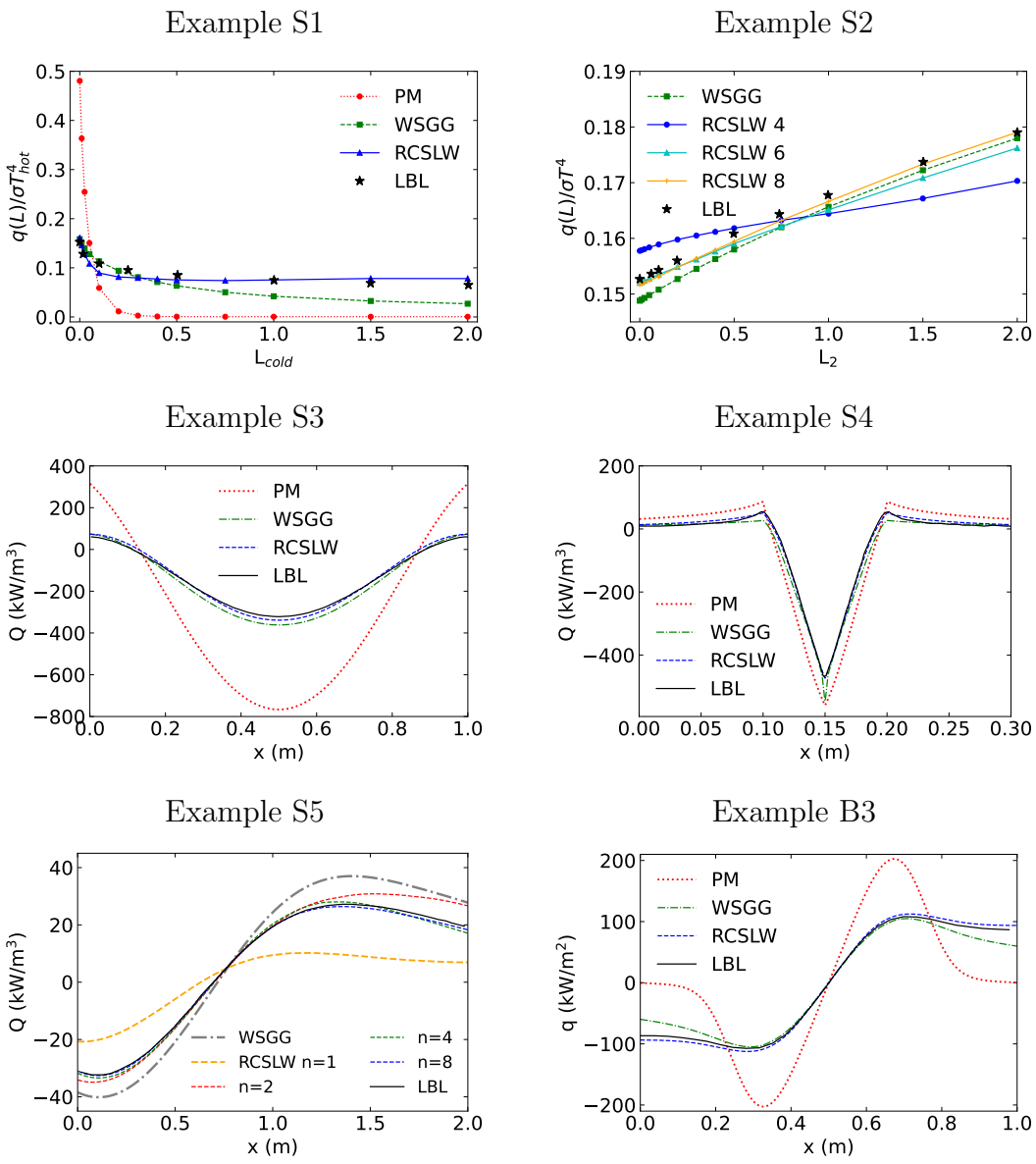

Figure 2: Results for Examples S1-S5 and B3 summarized in Table 1.

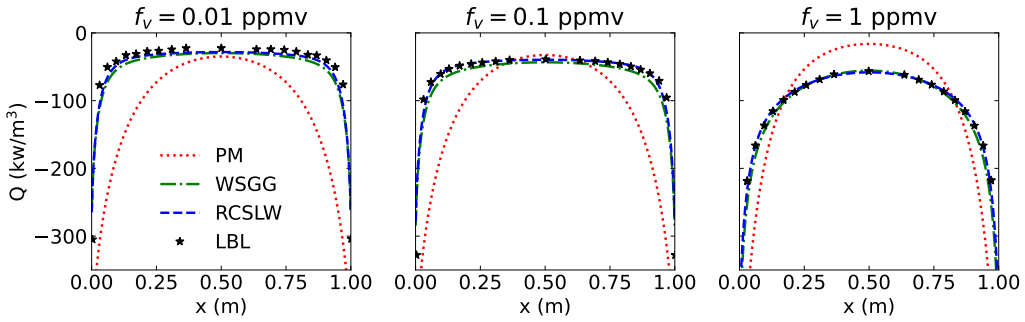

Figure 3: Results for Example Sb1 summarized in Table 1.

In general, the PM model performs poorly compared to the WSGG and RCSLW models and the LBL data. The results show that the PM model tends to exaggerate the trends displayed by the other models. The PM data mimics the shape of the other curves in Example S5 as well, but the curve is off-scale and omitted for clarity. For the PM model in Example S5, Q varies from around -80 kW/m^3 at $x = 0$ to a peak of 200 kW/m^3 at x=1.5 m and drops to 100 kW/m^3 at $x = 2$ m. In Example S2, the PM value of $q(L)/\sigma T^4$ is off the scale at an essentially constant value of unity. The PM absorption coefficient is 27.4 atm^{-1}m^{-1}, which results in a calculated optical thicknesses of 0.09 and 0.36 m in the thick and thin layers, respectively. These values are small compared to the domain sizes greater than 0.5 m considered in Example S2. Example S3 illustrates that the PM model tends to overpredict radiative heat loss at hight temperatures, which has been previously observed [10–12].

The WSGG model closely follows the trends of the LBL data for all examples, and in most examples gives reasonable quantitative agreement. This is especially true for Example S2, S4, and B3. For example S5, the WSGG model shows peak errors of around 50%, and somewhat higher in Example S1. The heat flux near the boundaries in Example B3 is low by around 30%. The RCSLW model gives results in very close agreement to the LBL data for all examples. A notable exception is example S2, where the heat flux at the right boundary is not well-predicted for four gray gases. The heat flux does converge to the LBL results when the number of gray gases increases. This behavior was not discussed in [17] where 24 gray gases were

used. The WSGG model is very close to the LBL data for this case. The good agreement is likely a result of the simplicity of this case that is isothermal with pure CO_2 at uniform concentration in either of the two adjacent gas slabs. The RCSLW model is sensitive to the number of gray gases used, as illustrated in Figure 2 by Examples S2 and S5. The difference in accuracy between $n = 2$ and $n = 8$ gray gases is small for all of the example cases (not shown) and typically falls within the margin of error represented by the WSGG model's deviation from the LBL data. The RCSLW model also depends on the value of the chosen reference temperature that is used to set the ALBDF grid. In Example S5, the RCSLW model does not converge to the LBL data at $x > 0.5$ m when the domain average temperature is used.

Figure 3 shows the results from Example Sb1, which considers three magnitudes of the soot volume fraction in addition to the radiating gas. Both the WSGG and RCSLW models perform accurately in all three cases, but the PM model displays significant deviations from the LBL data. In sooting flames, soot acts as a significant source and sink of radiation, and its radiative properties differ significantly from those of the participating gaseous species. Soot reactions and transport are both sensitive to, and strongly influence local variations in, flame temperature and gas composition, forming a feedback loop in which accurate prediction of both gas and soot radiative properties becomes critical to predicting flame properties and behavior, particularly late-stage flame phenomena such as flame sheet breakthrough, smoke production, and extinction and reignition processes.

5.1. CFD Results

The RadLib model was coupled to the Fire Dynamics Simulator (FDS) code developed at NIST [20]. FDS is written in Fortran, and the Fortran interface of Radlib was used for simulations. FDS includes several radiative models, but the spectral WSGG model coupled to a finite volume discrete ordinates model is used here. This was done by editing the `radi.f90` file. A `use rad_module` statement is included and the functions `A_WSGG` and `KAPPA_WSGG` were replaced with calls to RadLib's `get_k_a_oneband`. The `oneband` version was used because FDS does an outer iteration over the bands/gases, computing properties at a given band for each grid point.

FDS includes a number of validation cases. Here, we compare to the FM Burner case. The configuration is a vertically fired gas burner with various fuels and with a coflow oxidizer stream of varying nitrogen dilution. The burner has outer and inner diameters of 15.2 and 13.7 cm, respectively, and

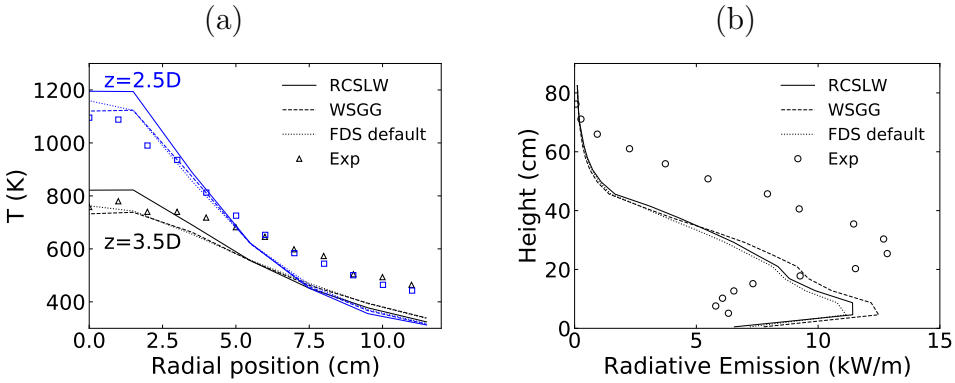

Figure 4: Radial profiles of mean temperature at two heights (a), and height versus radiative emission (b) for FDS simulations of the FM Burner validation case comparing three models to experimental data.

is near the floor in the center of a 1.22 by 1.22 by 1.83 m tall compartment. The heat release rate was 10 kW and included a 1 kW pilot in a surrounding ring. The coflow oxidizer was fed through the floor. Simulations performed here used the ethylene fuel with 20.9% N_2 oxidizer (i.e., air). Further FDS model and case simulation details are provided in the FDS validation and user guides [20].

Figure 4 shows results of the simulation with comparison to experimental data. Three radiation models were included: the FDS default model, and the RCSLW and WSGG models from RadLib (both using four gray gases and one clear gas). The FDS default model uses a single gray gas with a composition and temperature dependent absorption coefficient computed from RADCAL. Further details are provided in the FDS user guide [20]. Figure 4a shows radial profiles of mean temperature at two vertical positions. The models produce centerline temperature differences of about 80 K (7%) between the RCSLW and the WSGG at z=2.5D, and 90 K (12%) at z=3.5D. The differences are lower at lower points in the flame since the effect of radiation on temperature is cumulative. Figure 4b plots height versus radiative emission per unit length along the centerline with the spread in radiative emission around the peak values being 1.3 kW/m (11%).

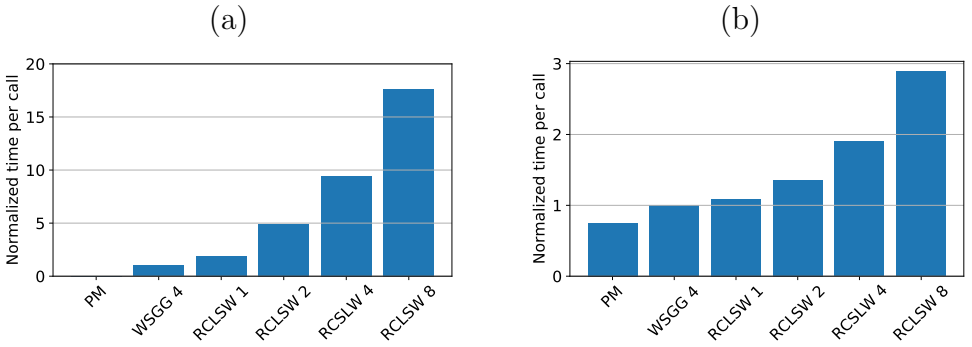

Figure 5: Relative computational cost to (a) evaluate gas properties only and (b) run Example S3, including the ray-tracing solver. Results are normalized by the cost of the WSSG model for each case.

5.2. Computational Cost

In addition to comparing model attributes and performance, we evaluated and compared the computational cost of the implemented radiation property models. Calculations were performed on a 4 GHz Quad Core Intel Core i7 iMac, version 10.15.7. The results, normalized by the cost of the WSGG model, are summarized in Figure 5. In the results presented, only the cost of evaluating the solution was included; model initialization and input/output costs were neglected. In the results including the ray-tracing solver, the same number of rays and grid points is used in all calculations.

Figure 5a displays the relative cost to compute the gas properties κ and a, represented by the time required to execute the C++ function `get_k_a()`, averaged over one million evaluations. The results for each model are normalized by the WSGG model, which required an average of 8.0E-7 s. Relative to the WSGG model, the cost to evaluate the gas properties with the PM model was 0.098. The RCSLW model was evaluated with $n = 1$, 2, 4, and 8 gray gases, which resulted in relative costs of 1.9, 4.9, 9.4, and 18, respectively, which is very nearly proportional to the number of gray gases considered.

Figure 5b shows the cost to evaluate Example S3, which involves both evaluation of the gas properties and solution of the RTE using the provided ray-tracing solver. This is relevant because radiative property calculations are rarely done in isolation, but are part of a larger RTE solution, so that overall cost differences may be smaller than those of the property evaluations alone. This is consistent with the results of the figure and as follows.

Relative to the WSGG model, which required 0.0079 s, the model costs for the PM model and the RCSLW model with $n = 1$, 2, 4, 8 gray gases was approximately 0.75, 1.1, 1.4, 1.9, and 2.9, respectively.

Cost comparisons were also attempted with Python, but meaningful results are difficult to obtain when mixing Python and C++. In particular, the cost of a single evaluation of the gas properties is small and evaluating the gas properties in a Python loop results in the loop itself appearing to dominate the computational cost. Comparison between Python and C++ for Example S3 is somewhat more meaningful, but even here, for the six cases considered in Figure 5 the cost only varied by about 4%, indicating that the computational cost is dominated by Python wrapper rather than by the underlying C++ model evaluations or solver. The cost of the WSGG model was 0.6 s, which is 7.6 times slower than the C++ version. It is possible that optimizing the Cython interface could improve the speed and relative cost of using Python with RadLib, but RadLib's Python interface and examples are primarily intended to demonstrate the library's use and provide a convenient interface rather than serve as a point of use for detailed CFD calculations.

6. Conclusions

Radiative heat transfer phenomena are historically difficult to model and implement in CFD calculations due to their high level of conceptual and mathematical complexity and potentially large computational cost. Many combustion CFD studies either neglect radiative heat transfer or employ oversimplified models that do not accurately represent combustion systems. Most combustion processes of interest to engineers and researchers, however, involve significant radiative heat transfer, and simulations require robust radiative modeling, which includes both radiation property modeling and solution approaches for the radiative transfer equation to yield accurate results.

RadLib is a C++ library of radiation property models developed to facilitate implementing radiative property models in CFD simulations. At present, it includes three major radiation property models—Planck Mean (PM) absorption coefficients using the optically thin approximation, the weighted sum of gray gases (WSGG) model, and the rank-correlation spectral line weighted-sum-of-gray-gases (RCSLW) model. Each of the implemented models has been validated and the library's structure and functionality has been outlined. The library can be expanded to include additional property models.

In addition to the library itself, RadLib includes several illustrative example cases in a one-dimensional parallel planes geometry using a simple ray tracing solver to demonstrate use of the library and validate model implementation. Results are compared to line-by-line (LBL) solutions. In general, the RCSLW model outperforms both the PM and WSGG models in terms of accuracy at the expense of computational cost.

RadLib is intended as a convenient access point for researchers who require radiation property modeling tools for relatively high temperature CFD applications, such as combustion, but could potentially be applied to research problems involving radiative heat transfer in other fields as well. RadLib is designed to facilitate and simplify the process of implementing and/or using radiative property models; it consolidates various model types into a single library with a consistent framework, reducing some of the overhead associated with choosing, implementing, and testing radiation property models. Its framework can be used to implement and validate new models as well as compare existing models under consistent conditions. By facilitating model comparison through a common interface, RadLib can provide a practical means of testing specific modeling approaches without the restrictions imposed by large-scale CFD simulations.

7. Declaration of Competing Interests

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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