COMPUTATIONAL METHODOLOGIES

FOR THERMAL RADIATION MODELING

By

NICOLAS TRICARD

A thesis submitted to the University of Connecticut for the degree of MASTER OF SCIENCE

Computational Thermal Fluids Lab

Department of Mechanical Engineering

School of Engineering

University of Connecticut

December 2022

ACKNOWLEDGMENTS

Insert acknowledgements here.

Table of Contents

List of Figures

List of Tables

ABSTRACT

Insert abstract here

Chapter One

Introduction

Over 80% of energy produced on earth is produced through combustion. Adequate understanding of combustion requires modeling of thermal radiation in order to capture the high heat flux values transported through the domain.

The seminal equation for thermal radiation is the Radiative Transfer Equation (RTE), eq. ??.

$$\frac{dI}{ds} = \dot{s} \div I \tag{1.1}$$

1.1 Motivation

The immense computational expense required for integration of the multitude of coupled equations within a combustion simulation are infeasible even with modern computing resources. In particular, radiation becomes prohibitive due to its all-to-all nature.

In attempt to maximize accuracy at the limitations of present resources, a number of models have been introduced to reduce the computational burden of radiation modeling. Of those, many involve complex mathematical assumptions and simplifications which can be difficult to learn, account for, and may lead to inaccurate results for many circumstances.

Of those, the Monte-Carlo Ray Tracing (MCRT) method stands out as the most robust.

MCRT is a direct physical interpretation of physical process by which the rays are transported through space. Within MCRT, random rays are initiated within the computational cells of the combustion simulation, and are tasked with traveling in a

- 1.2 Importance of soot and radiation in fire spread
- 1.3 Buoyancy-driven diffusion flames
- 1.4 Data-based approach
- 1.5 Organization

Chapter Two

Models and Methods

0 1	α	1 .	
2.1	Soot	physics	3
4 • 1		PILY DIC	J

- 2.1.1 Soot formation
- 2.1.2 Soot growth and destruction

2.2 Soot models

Soot model expectations

Difficulties in soot modeling

2.2.1 Classification of soot models

Empirical soot models

Semi-empirical soot models

Detailed soot models

- 2.2.2 Review of soot research
- 2.2.3 Soot models used in the present work

Two-equation model

2.3 Soot modeling sensitivity

- 2.3.1 Chemical mechanisms
- 2.3.2 Precursor species
- 2.3.3 Reaction rates

Chapter Three

Ch3

Chapter Four

Data Assimilation

4	-1	T			1	, •	,
		In	tr.	α	111	ct 1	ion
+.				. , , ,			

4.1.1 Kalman filters

Kalman filter

Ensemble Kalman filter

Other filters

Previous studies

4.1.2 Organization

4.2 Toy problem and parametric study

4.2.1 Baseline solution verification

4.2.2 Parametric study

Ensemble size

Model and measurement noise

Assimilation frequency

4.3 Formulation for a coupled flame simulation

4.3.1 Localization

4.3.2 EnKF algorithm

4.4 Soot model tuning

Chapter Five

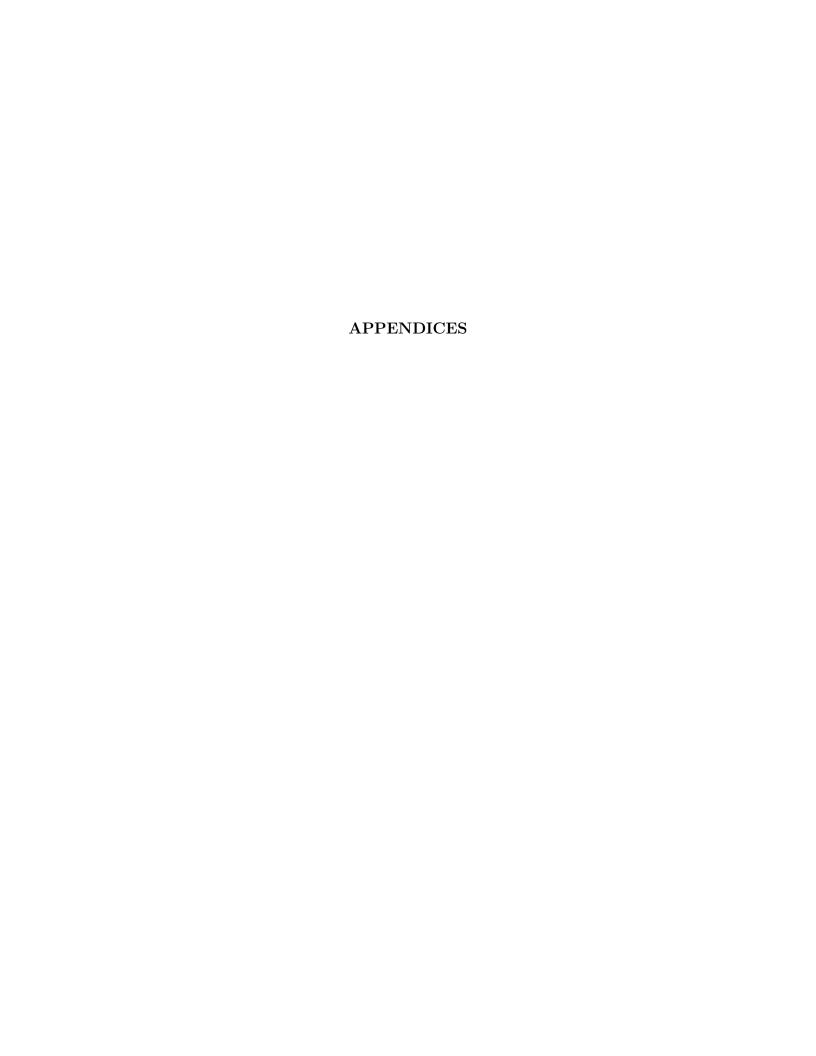
Machine Learning Approach

5.1 Introduction

Chapter Six

Conclusions and future work

6.1 Summary of findings



Appendix A

Data assimilation Supplementary

Material

A.1 Appendix Section 1

Temperature

Sample text

Soot volume fractions

Sample Text.

A.1.1 Assimilation of soot volume fraction measurements

Sample text

A.2 Source term implementation

Sample text.

Appendix B

Machine Learning Supplementary

Material

B.1 Parametric study of the penalty coefficient

Sample text