UNIVERSIDAD POLITÉCNICA DE MADRID
ESCUELA TÉCNICA SUPERIOR
DE INGENIEROS DE TELECOMUNICACIÓN

**STUDY, DESIGN AND VALIDATION OF A
FRAMEWORK MODEL FOR SMOKE AND
PARTICLE-FILLED ATMOSPHERES**

PhD Thesis

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This one goes out to the ones I love

*"The best scientist is open to experience
and begins with romance - the idea that
anything is possible."*

Ray Bradbury

*"diu venturus erat et ibi
est multus labor faci"*

(it has been a long time
and there is still
much work to be done)

Commercial systems are presented or used throughout this work,
and it should not go without saying that their mention does not
present any form of endorsement by the author.

Resumen

La visión es el sentido que aporta la mayor cantidad de información sobre conciencia situacional en humanos. Esto es relevante en el caso de pérdidas temporales de visión por parte de profesionales por sus implicaciones en seguridad –en especial durante la realización de tareas de riesgo–. Esta tesis aporta una serie de contribuciones para facilitar el desarrollo futuro de dispositivos capaces de solventar los riesgos y problemas asociados a ese tipo de ceguera temporal.

En primer lugar se da una visión general de concepto desde una perspectiva de teledetección. Se analiza el estado del arte de varias tecnologías en uso hoy en día en aplicaciones relacionadas con la pérdida de visión en entornos exigentes. Se estudian sus posibilidades desde un punto de vista teórico, así como desde el punto de vista del usuario para determinar ventajas, inconvenientes y posibles áreas de mejora.

A continuación se estudian los aspectos teóricos y prácticos de distintos tipos de señal y su aplicación a los sistemas de visión artificial, analizando su adecuación a la obtención de imágenes en medios tales como las atmósferas con partículas en suspensión. Se realiza una comparación entre ondas electromagnéticas y de presión como medios de detección del entorno, extrayendo conclusiones que apuntan a la necesidad de explorar nuevas tecnologías para mejorar el rendimiento de los sistemas actuales. Se definen dos casos de estudio, uno relacionado con operaciones de extinción de incendios y el otro con operaciones subacuáticas de baja visibilidad.

La caracterización del medio perturbador se identifica como la piedra angular en la modelización de la propagación de la señal a través de atmósferas con partículas en suspensión. En ese sentido, se realiza un análisis en profundidad del humo como medio de propagación. Se caracteriza el humo como una suspensión de partículas en una atmósfera con una cantidad variable de productos de combustión. Además, se estudia junto con sus características principales: tamaños de partícula, propiedades ópticas, movimiento, etc. Se define un conjunto de parámetros válido para alimentar un modelo. A continuación se generalizan esas características a otros entornos –como aguas turbias–, aunque el presente trabajo se centre en atmósferas con humos.

Con el medio completamente caracterizado, es posible crear un modelo de Monte Carlo basado en eventos para describir las interacciones entre una radiación electromagnética incidente y una atmósfera con partículas en suspensión.

El modelo está concebido como un modelo marco: es posible simular una amplia variedad de entornos con partículas en suspensión de tipos y propiedades arbitrarias sin grandes cambios. Se incluye también la definición del entorno espacial. A pesar de estar inicialmente pensado para longitudes de onda ópticas y de infrarrojos, es posible generalizar el modelo a otras partes del espectro. Este modelo, junto con la metodología de caracterización del medio, suponen la contribución original principal de la presente Tesis Doctoral.

A continuación, se presenta y se discute la implementación del modelo en una arquitectura con alto grado de paralelización. Se realiza también la identificación de sumideros de rendimiento, y se analiza el hardware subyacente para la optimización del rendimiento.

Se llevan a cabo dos estrategias de implementación, extrayendo consejos prácticos para maximizar la efectividad de las optimizaciones implementadas. La vasta cantidad potencial de datos generados por el modelo hace conveniente la existencia de algún tipo de herramienta para el análisis rápido y la explotación de los resultados obtenidos. En este marco se ha desarrollado una herramienta de visualización gráfica como prueba de concepto y que ha resultado ser de gran utilidad práctica.

Finalmente, se diseñó y construyó un experimento para la validación del modelo con pruebas reales. Se explora también el flujo de trabajo necesario para conseguir el diseño rápido de un instrumento coste-efectivo para la realización de los experimentos. Para ello se usaron técnicas de diseño avanzado como el diseño paramétrico. El instrumento se fabricó usando técnicas de fabricación aditiva (impresión en 3D), incluyendo un método original para inyectar y confinar el medio en una cámara construida a propósito. Adicionalmente, se diseñó y probó un procedimiento para crear atmósferas estables y reproducibles a nivel microscópico usando microesferas calibradas. Dicho procedimiento es una contribución original del presente trabajo.

Se realizaron varios experimentos de los cuales se obtuvieron los pertinentes resultados. En esta primera fase se obtuvieron datos cualitativos que mostraban buena correlación entre las simulaciones y los experimentos. Debido a la capacidad del hardware usado, la obtención de datos numéricos precisos se deja como trabajo futuro, junto con la exploración de –entre otras–, las técnicas de *compressed sensing* para el procesado de señal.

Abstract

Vision is by far the most important source of information regarding situation awareness in humans. This is relevant in the case of temporary loss of vision for certain professionals due to safety implications –specially when conducting exposed tasks–. This thesis makes a number of contributions to facilitate the future development of devices able to overcome the risks and problems related with that kind of temporary blindness.

First, a concept overview of the problem from a remote sensing perspective is given. An analysis of the state of the art of several technologies used today in applications involving loss of vision in harsh environments is conducted. Their possibilities are studied from a theoretical point of view as well as from the user's perspective in order to determine advantages, disadvantages and possible areas of improvement.

The theoretical and practical aspects of different signal domains and their application to artificial vision systems are studied next, surveying their suitability to imaging in media such as particle-filled atmospheres. A comparison between electromagnetic and pressure waves as a means of sensing the environment is made, extracting conclusions pointing to the need to explore new technologies to enhance the performance of current systems. Two cases of study are defined, one related to fire suppression operations and another one to low visibility underwater operations.

The characterization of the disturbing medium is identified as the cornerstone in the modeling of signal propagation through particle-filled atmospheres. In that sense, an in-depth analysis of smoke as a propagation medium is carried out. The characterization of smoke as a suspension of particles in an atmosphere with a variable degree of combustion products is conducted. Main characteristics of smoke are also studied: particle sizes, optical properties, motion, etc. A reference set of parameters to feed a computer model is defined. Next, the generalization of those characteristics to other environments such as turbid water is done, although the present work is more focused on smoke-filled atmospheres.

With the medium completely characterized, it is possible to create an event-based, time resolved Monte Carlo model to describe interactions between an incident electromagnetic radiation and a particle-filled atmosphere. The model is conceived as a framework model: a wide scope of particle-filled environments with arbitrary particle types and optical properties can be simulated without ma-

for changes. The definition of spatial environments with objects is also included. Although primarily intended for use in optical and infrared wavelengths, the model can be generalized to other parts of the spectrum as well. This model, along with the characterization of the medium, are the main original contribution of this PhD thesis.

The implementation of the model in a highly parallel computer architecture for higher performance is presented and discussed subsequently. The identification of performance drainers, and the analysis of the underlying hardware for performance optimization have been worked out.

Two implementation strategies were used and analyzed, extracting practical hints to maximize the effectiveness of the optimizations implemented. The huge amount of data generated potentially by the model makes it convenient to have some sort of tool for rapid analysis and exploitation of the results obtained. A visual tool has been developed as a proof of concept, and has proven to be very useful in practice.

Finally, an experimental setup was designed and built to validate the model against real world tests. The workflow necessary to provide with a rapid design of a cost-effective instrument to run the experiments was planned, making use of advanced techniques such as parametric design. The instrument was fabricated using additive manufacturing techniques (3D printing), and included a way to inject and confine the medium inside an ad-hoc built chamber. A procedure to create stable and reproducible atmospheres at a microscopic level using calibrated microspheres was also designed and tested, accounting for an original contribution of the present thesis.

Several experiments were run and results were obtained. In this first phase of the experiments, qualitative data showing good agreement between simulations and experiments was obtained. Due to the capabilities of the hardware used, the obtention of accurate numerical data is left for future work, along with the exploration of –among others–, compressed sensing techniques for signal processing.

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List of Acronyms

ADC	Analog-to-Digital Converter	138
AED	Aerodynamic Effective Diameter	65
APD	Avalanche Photodiode	50
ASTM	American Society for Testing and Materials	63
CCD	Charge-Coupled Device	153
CDF	Cumulative Distribution Function	89
CFD	Computational Fluid Dynamics	85
CIE	International Commission on Illumination	12
CIS	CMOS Image Sensor	153
CMOS	Complementary Metal–Oxide–Semiconductor	138
CNC	Computer Numerical Control	157
CS	Compressed Sensing	174
CUDA	Compute Unified Device Architecture	118
CW	Continuous Wave	26
DIY	Do It Yourself	136
DMD	Digital Micromirror Device	178
DSP	Digital Signal Processor	24
EEA	European Environment Agency	64
EPA	Environmental Protection Agency	64
EVA	Ethylene Vinyl Acetate	153
FIR	Far infrared	13
FLIR	Forward-looking infrared	13
FOM	Figure of Merit	31
FOV	Field Of View	53
FPGA	Field-programmable Gate Array	24
GPGPU	General-Purpose GPU	117
GPIO	General-Purpose Input/Output	157
GPU	Graphic Processing Unit	117
GSD	Geometric Standard Deviation	66
IIR	Intermediate infrared	13
IR	InfraRed	13
ISO	International Organization for Standardization	12
LASER	Light Amplification by Stimulated Emission of Radiation	34
LED	Light-Emitting Diode	138
LIDAR	Light Detection And Ranging	47

LWIR	Long-wavelength infrared	13
MEMS	MicroElectroMechanical Systems	53
MFP	Mean Free Path	88
MMAD	Mass Median Aerodynamic Diameter	66
MPE	Maximum Permissible Exposure	51
MRI	Magnetic Resonance Imaging	176
MWIR	Mid-wavelength infrared	13
NETD	Noise Equivalent Temperature Difference	16
NFPA	National Fire Protection Association	16
NIR	Near-infrared	13
PAH	Polycyclic Aromatic Hydrocarbon	62
PCB	Printed Circuit Board	155
PCX	Plano ConveX lens	146
PLA	PolyLactic Acid	156
PWV	Precipitable Water Vapor	45
PZT	Lead Zirconate Titanate	33
RGD-FA	Rayleigh-Gans-Debye-Fractal-Aggregate	76
RGD	Rayleigh-Gans-Debye	76
RIP	Restricted Isometry Property	176
RMS	Root Mean Square	79
RNG	Random Number Generator	120
SM	Streaming Multiprocessor	130
SMT	Surface-Mount Technology	157
SONAR	SOund NAvigation and Ranging	18
SWIR	Short-Wavelength InfraRed	13
TEM	Transverse Electric and Magnetic	38
TIC	Thermal Imaging Camera	16
TOF	Time-Of-Flight	51
TRM	Time-Reversal Mirror	56
UVM	Unified Virtual Memory	118

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1. Introduction and Motivation

"Something is happening. We are becoming a visually mediated society. For many, understanding of the world is being accomplished, not through words, but by reading images."

*Paul Martin Lester,
"Syntactic Theory of Visual
Communication"*

For the last two million years, humans and their precursors have been interacting with the environment using their senses. As it happens with higher primates like chimpanzees, early humans relied more on hearing and smell than we do today, where it is said that 83% of what we learn comes through vision [20]. This fact yields a very specific interaction between human subjects and their environment [21]. Far from focusing on increasing the amount of information received by other senses, society and media tend to deepen this dependency [22, 23].

So the first question to be asked would be: *why is the human being so prone to rely on visual stimuli to interact and get information about his environment?*. This question has been addressed in several studies (see for instance [24, 25]). Researchers have pointed to the strong relationship between vision and spatial perception as one of the strongest reasons why we rely so much in vision to explore and sense the space around us. Some authors have studied related topics such as the spatial perception in visually impaired or early blind subjects [26, 27], but their conclusions in these and other works are somewhat divergent. Explanations may be given on a wide range of terms, but in short there are subjective parameters inherent to dealing with perception, a fact that influences –if not determines– the dispersion of the results across different studies.

Hermann von Helmholtz and the Gestalt School have been credited with the first “modern” studies on visual perception [28]. Von Helmholtz concluded that optically, the eye was so poor, that there had to exist some form of unconscious inferences, that is, assumptions on previous experiences that completed the data gathered by the naked eye. These assumptions include:

- Light comes from above.
- Objects are normally not viewed from below.

- Faces are seen (and recognized) upright.
- Closer objects can block the view of more distant objects, but not vice versa.

Although the details of visual perception remain a subject open for research, there is clear evidence of the importance of vision in sensing the spatial environment of the individuals. This fact raises another important question, *what happens, then, when there is no vision available?*. The wide formulation of the previous question groups, on the one hand, visually impaired subjects (either blind or not), and on the other hand subjects who are temporary blind.

The original research interest that motivated the pursue of this thesis focused on the second group of subjects, and more precisely on persons that *can* see in their daily life but have to deal with situations where they become temporary visually impaired (such as military, professional divers, search and rescue operations staff, and others). Next section will introduce the topic in more detail.

1.1. Temporary visual impairment

The lack of vision leads automatically to a sudden loss of spatial perception. This fact, together with the relative “oblivion” of the rest of the senses results in an important lack of information about the environment, which, in turn, can make the subject feel uneasy, reducing his perception of safety and increasing stress levels. Many studies have been conducted in order to assess the influence of working conditions for high-risk workers in an aggregated manner [29, 30]. These works analyze physiological parameters like heart rate and ventilation (air consumption) of trained subjects in real-world situations to infer health related problems and propose workarounds as well as a number of recommendations. More modern research has led to the development of devices capable of triggering an alarm if the subject under monitorization is in danger [31].

Should measurable conditions like heat, pressure, unbreathable atmospheres, heavy duty jobs, exposure to chemicals or other factors of stress put pressure onto subjects’ bodies, other not-so-easy to measure conditions such as loss of vision, uncertainty, the existence of small cavities, lack of previous knowledge of the environment, etc. add to the psychological part of stress [32, 33]. These factors will contribute to physical stress in the end.

However, it is not easy to find significant research on the effect of temporary blindness linked to certain professional activities. Despite being acknowledged for many years, it has not been part of regular training of affected workers until recently [34].

It is of utmost importance to cope with temporary loss of vision since proper training and equipment in these situations, specially when dealing with harsh environments at an unknown location may mean the difference between life and

death. In fact, stress tests are part of selection procedures of personnel whose work is to be done under these circumstances¹.

The increase in stress and danger associated to these high-stress situations can be mitigated twofold:

- **Competence Training:** proper training can lower the stress when dealing with these situations by exposing the subject to similar, controlled situations in order to increase his “situation awareness”. This exposure helps subjects deal with extreme situations through special procedures and protocols: that is, training helps avoid mental blockage or panic in extreme conditions.

Another complementary approach is to increase the relative importance of other senses (smell, touch,...) through proper training. This is the approach used by blind people. They train their haptic, hearing and touch senses to partly compensate for the loss of vision. Some people have even developed “new” senses such as echolocation [36], which will be discussed later. Proper training is desirable since it will work in any circumstances; even in the case of failure of the equipment, personnel will be able to make use of the techniques learnt in order to manage the situation. This approach is practically unfeasible for large number of individuals (when they do not need this skill in their daily life): the time required to train all the staff at the required level may be incompatible with the work itself. This is the reason why some of these techniques are being developed with blind people in mind.

- **Product Design:** It is possible to make use of technology to minimize the effects of temporary blindness. For instance, firefighters have the aid of thermal imagers and other specialized gear to cope with the lack of vision due to smoke.

A combination of the two procedures above provides with the best solution. This thesis will make a number of contributions that will help develop new technologies whose final aim would be to overcome problems related to loss of vision.

1.2. Remote sensing systems for artificial vision

As stated in the previous section, research and development of technologies and devices is an approach that, when used in combination with proper training, can yield very good results.

These days, despite the technological advances already in use, it is wise to go

¹NFPA 1001 standard identifies the minimum job performance requirements for career and volunteer fire fighters whose duties are primarily structural in nature in the USA [35]. Candidate Physical Ability Test (CPAT) has been adapted and locally implemented by Fire Services in Madrid and in other Spanish cities in the recent years.

back to mother Nature to look for answers. Indeed, millions of years of evolution and biodiversity across different ecosystems and environments makes us think that problems that researchers try to solve may already be solved in Nature, usually in a very smart way. Taking Nature as an inspiration can give very interesting results. For instance, senses are way richer and more diverse in animals than in humans. The traditional “five human senses” proposed by Aristotle [37] –vision, hearing, smell, taste, and touch– are a small subset of other senses found in the wild providing with information about the environment:

- **Human senses:** balance and acceleration (position and direction, movement), temperature, proprioception (relative positions of body parts), time, etc.
- **Non-human senses:** vomeronasal (detection of pheromones), gravity (direction of grow in plants), electroreception (detects electric fields like the ones prey originate when contracting muscles), magnetoception (direction of flight by comparison with Earth’s magnetic field), pressure detection, current detection (lateral line in fishes used for navigation and schooling), polarized light detection (orientation of bees and other animals), slit *sensillae* (in insects, information about force and vibration from mechanical stress in the exoskeleton), echolocation (navigation of bats in the dark) and others.

After an overall study of the different abilities of animals in the wild that may have overcome the problems derived from very little or lack of vision at all, there are two groups of animals that are relevant to this work: bats (and dolphins) and troglobites.

Troglobites are animals that complete their life cycle inside a cave. They live in absence of light and therefore have developed senses that substitute vision. Such adaptations include a heightened sense of hearing, touch and smell in the form of longer antennae or legs, and lack of eyes, wings or pigmentation [38]. It is believed that they can measure slight changes in air pressure, humidity or temperature; from these measurements they can infer the position and even movement of other animals nearby.

On the other hand, bats (and dolphins) make use of what is called **echolocation**. Echolocation, also called biosonar, is the biological sonar used by several kinds of animals. Echolocating animals emit calls out to the environment and listen to the echoes of those calls that return from various objects near them. They use these echoes to locate and identify the objects nearby. This sense is used for navigation and foraging (or hunting) in various environments.

Echolocation [39] has been widely studied and is therefore more known than the senses of the troglobites. Both approaches share that they can “see” their environment (that is, gather information about the physical properties of their surrounding space, including objects or living species inside it) *sensing it all remotely*. Bats send ultrasound FM chirps that their specialized brain interpret in

Fig. 1.1.: Remote sensing system showing its fundamental parts: 1. Device. 2. Emitter. 3. Medium. 4. Objects. 5. Receiver.

real time, giving them accuracies in the range of or even under one millimeter [40]. This same sense is present in other species such as dolphins and other mammals [41, 42].

Figure 1.1 shows a scheme of a remote sensing system for artificial vision. A parallelism can be easily made with echolocating animals or even with human visual perception. The different parts of the system depicted in the figure can be explained as follows:

1. **Remote sensing device.** This device is responsible for the preparation of the signals to be emitted and for the postprocessing and presentation of the “visual” data to the user. It would be the equivalent to our brain.
2. **Emitter.** It emits the adequate signals for the particular medium and objects to be sensed. It is the “illuminating source”, and therefore it would be the equivalent to the sun or artificial light illuminating the object.
3. **Medium.** It is the intervening substance through which signals travel. It can be responsible for the underperformance or inability of the sense of sight to work properly, as the electromagnetic waves at optical frequencies (light) may not be able to traverse the medium or traverse it with so much degradation that makes it impossible for the brain to perceive the object. The performance of the system will be affected by the medium and the properties of the object –at the frequencies and remote sensing technology chosen–.
4. **Objects.** They are part of the space surrounding the device (and thus the user) and constitute the elements to be detected by the system. The ability of the system to form and present a recognizable image to the user will determine its subjective quality.
5. **Receiver.** It is the artificial element equivalent to the eye. In general, it will be responsible for collecting the radiation emanating from the object and thus affected by it after passing through the medium. The “sensed” radiation –raw data– is then sent to the remote sensing device for further processing.

The performance of the system is heavily dependent on the physical interaction

between the incident signal and the medium and/or objects. The range at which an object lays is related to the roundtrip time of flight of the incident signal and its velocity. Moreover, the particular interaction between the incident signal and the medium/objects may provide with further information about the object and/or the medium. These features will make concrete setups suit certain media and not others.

1.3. Problem statement and challenges

The basic idea would be to find ways to map the physical environment and present reliable information to the user to enable navigation and space awareness. The generation of images and their presentation to the user is an important subject that should be considered as well, since the more recognizable images generated by the system, the less training necessary for operating personnel.

The most relevant feature and challenge when it comes to propagation, detection and image reconstruction of a signal that has gone through “aggressive” media (such as smoke- or particle-filled atmospheres) is the *nonlinearity of the distortion* introduced by the particular medium. Remote sensing techniques have to deal with this type of distortion. The goodness of the artificial vision system will be highly related to its ability to overcome the changes introduced by scattering and other types of signal aberrations.

Signal processing techniques, as well as formatting or presentation (image formation) are independent to the signals used [43]: they are not affected by the underlying physical principles governing the physical propagation of the signals through the medium. Sensors, data acquisition and its early processing do depend on the physics behind and are therefore domain dependent.

1.4. PhD Objectives

As explained in the previous sections, there is a real need to overcome vision impairment in harsh environments for certain professionals. The main aim inspiring this PhD thesis could be enounced as follows:

“To pave the way for future devices relying on remote sensing to present the users with artificially generated images that increase their situation awareness and thus their safety while conducting exposed tasks in smoke, turbid water or other particle-filled atmospheres”.

As a first step in that direction, this thesis focuses on the characterization of the propagating medium and the creation of a model to predict signal propagation, this is, research and develop methodologies, systems and prototypes associated

with remote sensing for extreme environments and their application to smoke and other particle-filled atmospheres.

This general objective can be also expressed as the following set of objectives:

- Identify and exploit the constraints of the man-machine interface in extreme environments to detect key areas of research.
- Identify the constraints of the design of electronic devices for harsh environments in a comprehensive way, studying the theoretical performance of different approaches and types of signals.
- Model signal propagation through particle-filled atmospheres. This includes in-depth study of different dispersive media and their characteristics for their parametrization and description.
- Develop generalistic algorithms and models that describe dispersive and other disruptive media, including the development of software suites to simulate and exploit the data provided by the models, as well as optimization techniques to minimize run times that include advanced use and fine-tuning of GPUs.
- Design cost-effective approaches including rapid prototyping to validate and assess the accuracy of the data provided by the models developed.
- Create relevant knowledge internationally endorsed by relevant publications in prestigious media.

1.5. Contributions. Thesis overview

The main original contribution of this thesis is the framework model for the simulation of signal propagation through particle filled atmospheres presented in chapter 5. It makes it possible to obtain results for arbitrary environments, particle distributions and atmosphere configurations simulating interactions between incident radiation and discrete, individual particles and combining them. This model helps close the gap between scattering atmospheres considered in an aggregated, macroscopic manner, and particle Physics studies focusing on the interactions occurring at a microscopic level. The model provides with a set of tools that serves as the first step towards a complete software simulation tool to ease the development of devices and technologies for artificial vision in harsh environments.

Other original contributions are to be highlighted. First, the workflow used in the characterization of smoke has made it possible to generalize the parameterization of a smoke filled atmosphere to other media. Then, the method developed to create a truly “synthetic smoke” has provided with a simple method to obtain configurable and reproducible particle suspensions at a microscopic level assimilable to smoke that avoids the need for complicated setups needing actual

combustions.

In addition, a number of contributions involving integration of existing technologies or new uses of established procedures have been arisen along the way. For instance, the ones related to the implementation of the model or its validation using a custom designed and fabricated instrument. Last, the fundamental analysis of scattering and its relationship with different types of signals has proven important, as it reviews the literature on the topic from an Engineering perspective, extracting practical hints for the development of future technologies.

The contributions presented in this thesis can be enumerated in a per chapter basis as follows:

- In chapter 3:
 - An in-depth analysis of the theoretical and practical aspects of different signal domains and their application to artificial vision systems.
 - A comparison of electromagnetic and pressure waves as a means of sensing the environment.
- In chapter 4:
 - The characterization of smoke as a suspension of particles in an atmosphere with a variable degree of combustion products.
 - The study of the main characteristics of smoke (particle sizes, optical properties, motion, etc.) and the definition of a reference set of parameters in order to feed a computer model.
 - The generalization of those characteristics to other environments such as turbid water.
- In chapter 5:
 - The creation of an event-based, time resolved Monte Carlo model to describe interactions between electromagnetic waves and a particle-filled atmosphere.
 - The generalization of the previous model to arbitrary particle geometries (the creation of a framework model).
- In chapter 6:
 - An efficient implementation of the computation intensive model described in the previous chapter taking advantage of parallelization in a GPU.
 - The identification of performance drainers in a kernel and the analysis of the underlying hardware for performance optimization.
 - A comparison of manual optimizations of the code with the optimizations introduced automatically by the CUDA compiler.
 - The analysis of the profiling data obtained, extracting practical hints to maximize effectiveness of the optimizations implemented.

- The development of a visual tool to exploit and interpret the huge amount of data potentially offered by the model.
- In chapter 7:
 - The workflow necessary to provide with a rapid design of a cost-effective instrument to run real-world tests.
 - The complete design and fabrication of the prototype itself using additive manufacturing.
 - The creation of reproducible atmospheres at a microscopic level.

1.6. Publications

Some of the results and contributions presented in this thesis have been already published in the JCR-indexed journals listed below:

- Nadal-Serrano JM, Lopez-Vallejo M: **A Survey on Theoretical and Practical Aspects of Imaging Aids for Artificial Vision in Professional Environments**. *IEEE Sensors Journal* 2015, **15**(5):2719 – 2731.
- Nadal-Serrano JM, Lopez-Vallejo M: **A time-resolved Monte Carlo smoke model for use at optical and infrared frequencies**. *Fire Safety Journal* 2015, **71**:299 – 309.
- Nadal-Serrano JM, Lopez-Vallejo M: **A Performance Study of CUDA UVM versus Manual Optimizations in a Real-World Setup: Application to a Monte Carlo Wave-Particle Event-Based Interaction Model**. *IEEE Transactions on Parallel and Distributed Systems* 2016, **27**(6):1579 – 1588.

Two additional publications are currently under preparation.

1.7. Document structure

Chapter 1 serves as a general introduction, stressing the relevance of temporary loss of vision for certain activities considering its safety implications. A concept overview of the problem is given from a remote sensing system perspective.

Chapter 2 analyzes the state of the art of several technologies used today in applications involving loss of vision in harsh environments. Their possibilities are studied from a theoretical point of view as well as from the user's perspective in order to determine advantages, disadvantages and possible areas of improvement.

Chapter 3 is devoted to remote sensing. Different types of signals and their suitability to imaging in media such as particle-filled atmospheres is studied. Conclusions are then extracted, pointing to the need to explore new technologies to

enhance the performance of current systems.

Chapters 4, 5, 6 and 7 are devoted to the development of a framework model of signal propagation in certain harsh environments that could help design and simulate the performance of new technologies and prototypes. First, chapter 4 focuses on the definition and parameterization of highly disruptive media: smoke and mineral dust in underwater environments. Its properties and particularities are studied without loss of generality. Next, chapter 5 describes the model developed, its possible generalizations to other parts of the spectrum and types of particle-filled media. The implementation of the model in a highly parallel computer architecture for performance maximization is presented and discussed in chapter 6. Then, chapter 7 describes the early validation of the model developed, including the design and construction of the instrumentation used and the results obtained.

Chapter 8 provides with an introduction and some interesting thoughts on future research lines. Possible uses of new trends, focusing on compressed sensing techniques to enhance the performance of prospective remote sensing devices and applications in harsh environments are discussed.

The conclusions of the thesis are finally presented in chapter 9.

2. State of the art of existing systems. Cases of study

"If I have seen further it is by standing on the shoulders of Giants."

Isaac Newton,
"The Correspondence Of Isaac Newton"

This chapter presents the state of the art of existing systems in the field of remote sensing that may be of use for short-range mapping (tens of meters) in harsh environments involving particle-filled atmospheres. Two cases of study have been chosen as representative for their relevance in real-world environments. They will serve as a practical reference and as such they will be recurrently recalled through this text:

- Vision through smoke or dust for ambient and firefighting operations.
- Vision through floating sediment for underwater operations.

They both will be analyzed in the next sections.

2.1. Firefighting imaging systems

Low to no visibility is inherent to firefighting operations in structural fires. It is a very important issue specially when dealing with enclosure fires, remarkably in confined and underground infrastructure such as tunnels, metro stations and garages, just to name a few.

Proper training is, with the aid of proper equipment, the only effective way to reduce stress and increment objective safety in this high demanding scenario. Technology has evolved and new devices and protocols have been introduced through research [44, 45]

Although there are authors that have proposed other technologies [46], there is one that is so far the most widely used in this specific area: thermal imaging. Next section is devoted to it.

Fig. 2.1.: Infrared bands (©2011 HowStuffWorks.com).

Fig. 2.2.: Infrared subbands.

2.1.1. Thermal imaging

The concept of thermal imaging traces back to 1800 [47]: Sir William Herschel, a British astronomer, musician and scientist discovered that colors below red not visible to the naked eye were detectable if viewed through a prism. Those “calorific rays” were in fact thermal rays, which are the basis for today’s infrared (IR) imaging technology.

Infrared Spectrum lays between the visible and the terahertz band (see Figure 2.1). It has been classified and subdivided by several organizations like the International Commission on Illumination (CIE) [48] and the International Organization for Standardization (ISO) [49], although the most commonly used division can be seen in Table 2.1 and Figure 2.2 (following [50]).

Objects emit electromagnetic energy whose spectrum and magnitude depends directly on their temperature, following the Black Body [51, 52, 53] radiation. This physical property allows the development of sensors and ultimately specially crafted cameras to virtually “see” objects in total darkness.

Tab. 2.1.: Classification of IR Bands.

Band name	Band abbreviation	Wavelength (λ)	Description & Use
Near-infrared	NIR, IR-A DIN	0.75-1.4 μ m	Defined by the water absorption. Fiber optic telecommunication [low attenuation losses in the SiO ₂ glass (silica) medium]. Image intensifiers (night vision).
Short-wavelength infrared	SWIR, IR-B DIN	1.4-3 μ m	Water absorption increases significantly at 1450nm. The 1530-1560nm range is for long-distance telecommunications.
Mid-wavelength infrared	MWIR, IR-C DIN, called Intermediate infrared (IIR)	3-8 μ m	Guided missile technology: the 3-5 μ m portion of this band is used for passive IR “heat seeking” missiles.
Long-wavelength infrared	LWIR, IR-C DIN, sometimes “far infrared”	8-15 μ m	This is the “ <i>thermal imaging</i> ” region. Sensors can obtain a passive picture based on thermal emissions only. Forward-looking infrared (FLIR) systems use this area of the spectrum.
Far infrared	FIR	15-1000 μ m	

2.1.1.1. Black-body Radiation

The so-called black body or thermal emission is described by Planck’s Law [51] and depends only on object’s temperature and emissivity¹:

$$B_{\nu}(T) = \frac{2h\nu^3}{c^2} \frac{1}{e^{\frac{h\nu}{k_B T}} - 1} \quad (2.1)$$

where B is the spectral radiance, T is the absolute temperature of the black body, k_B is the Boltzmann constant, h is the Planck constant, ν is the frequency, and c is the speed of light. Planck’s law accurately describes black body radiation, proposing that electromagnetic radiation is emitted in quanta. Besides, it converges with the Rayleigh-Jeans law in the lower frequencies, and the Wien approximation in the higher frequencies.

The sun has an equivalent black body temperature of 6000K, which translates in a peak emission around 500nm, close to the middle region of the visible spec-

¹Emissivity affects how the thermal radiation intensity relates to the actual temperature. It does so in a way that can make the substance under observation appear to have a temperature different from reality. A substance having an emissivity of 1 is said to be a “blackbody”, meaning that it absorbs and re-emits all energy incident upon it, and thus is representative of its actual temperature. A surface or gas having an emissivity of 0 reflects all energy, making the surface or gas appear colder than it actually is.

Fig. 2.3.: Plank's law showing black-body radiation at room and fire temperatures.

trum (this is the reason why humans can see the sun). Objects at room temperature (around 300K, see Figure 2.3) have a peak in the infrared region, with wavelengths near $10\mu\text{m}$. This difference of wavelength (1:20) has an important impact on the behavior of infrared emissions compared to that of visible light in smoke or dusty conditions. See Section 3.2.2 and Figure 3.7 for a detailed explanation. At fire temperatures (450-900K for enclosure fires) thermal emission peaks are between 3 and $5\mu\text{m}$, well inside the MWIR band (as seen in Figure 2.3). Besides, infrared imaging has the advantage of providing with images similar to those obtained with visible light and thus easily interpretable by untrained personnel.

Smoke can include, among other things, soot, ash, polymers, solids and even liquids. Soot dominates the smoke of an open-flame fire. In the particular case of urban fires, smoke comes from incomplete burning of a variety of materials, ranging from metals to wood; from wool, cotton and other natural textile fibers to paint, polymers and many other oil derivatives. It is therefore clear that smoke from a mixture of those materials will contain particles of different sizes and compositions that will behave like an aerosol² (see [54] for a comprehensive study of aerosols and their dynamics).

The prospective application and the conditions under which infrared imaging

²Aerosol. A colloidal suspension of particles dispersed in air or gas.

Fig. 2.4.: Atmospheric transmission in the IR band. LOWTRAN simulation taken from [1].

is going to be used determine the most advantageous sensor to embed in a certain type of thermal camera. Moreover, the intrinsic conditions of the atmosphere and, in enclosure fires, the presence of molecules as combustion byproducts do affect thermal emissions. It is possible to run simulations that predict atmosphere transmittance for several ranges and altitudes using LOWTRAN [55] (see Figure 2.4).

The transmittance of the atmosphere, combined with the emission spectrum (black body) at fire temperatures condition the sensors used in thermal imaging.

There are two main types of **infrared detectors** (see [56] for more information): photonic and thermal.

- **Photonic:** in this type of sensor, photons with an energy higher than a given threshold generate free carriers in a photodetector. They are fast but some require cooling.
- **Thermal:** they rely on the heating effect of the incoming radiation. The heat flux changes a certain parameter in the sensor (resistance, capacitance, etc.) which is then converted into an electrical change and then measured. They do not need cooling but are rather slow (milliseconds).

Modern infrared sensors tend to “pixelize” the sensor building Focal Plane Arrays (FPAs) in which the sensing element is repeated to form a 2D sensing surface no matter which type of sensor.

For clear reasons, we will focus on uncooled systems whenever possible.

2.1.1.2. Bolometer detector technology

All thermal detectors are based on the same principle: a sensing element is heated by the incoming IR radiation [57]. That change in temperature is measured indirectly through the change in a certain electrical magnitude. In the case of bolometers, the magnitude that changes is resistance or capacitance (see Figure 2.5 for a patented microbolometer). Usual constitution materials are amorphous silicon (aSi) and vanadium oxide (VOx) because they need no cooling at all.

Fig. 2.5.: Microbolometer (adapted from [2]).

Bolometers [58] are a type of thermal detectors that today constitute the sensing element of many devices incorporating staring focal plane arrays. In terms of noise they have Noise Equivalent Temperature Difference (NETD) figures as low as 50mK, which makes them suitable for a wide range of applications. Bolometers are assembled forming arrays of –typically– 320x240 or 160x120 elements. As stated in [59], the detector output requires a correction based on reference points provided by a chopper.

2.1.1.3. Thermal Imaging Cameras (TICs)

Recent improvements in thermal imaging sensors such as aSi (amorphous silicon) bolometers have led to relatively lower prices and rapid widespread of Thermal Imaging Cameras (TICs) for civil applications in law enforcement and firefighting.

However, there is a variety of sensors (pyroelectric bolometers, non-pyroelectric ones, silicon-based, vanadium-based, etc.) which exhibit different responses to the same tests and therefore the images displayed can vary significantly from one model to another.

Firefighters may find open flames, smoke or sprays of water when conducting search-and-rescue tasks. It is important for thermal cameras to perform well under these circumstances. Most of the cameras are National Fire Protection Association (NFPA) [60] compliant and thus respond in the spectrum covering 8-14 μ m, suitable for Germanium optics and exhibiting high transmittance values. They also display a temperature measurement, which is only approximate since emissivities from all objects in the scene are supposed to be 0.95 (see [61] for a discussion on radiative heat transfer and black-body radiation).

The introduction of further signal processing techniques and their smaller size have led to a better acceptance by the fire community. Examples of different state-of-the-art thermal cameras are shown in Figure 2.6.

Fig. 2.6.: Examples of images taken with several TICs from different firms: (a) and (b) Bullard; (c) and (d) Dräger; (e) and (f) MSA.

2.1.1.4. Limitations of Thermal Imaging Cameras (TICs)

Despite the obvious advantages of using TICs for firefighting, they also have limitations [62]. Most of them come from the need for proper training:

- Images can be difficult to interpret accurately when based upon certain objects, specifically objects with erratic temperatures, very hot objects (haloing) or thermal inversions.
- False sense of safety may lead to taking higher risks.
- Little contrast in cold smokes and/or uniform temperature scenes.
- High price and strict regulations due to their dual-purpose nature³.
- Some may have it hard to operate under heavy rain conditions.
- They cannot see through glass or under water.
- Radiation can be reflected and produce ghost images.

In conclusion, TICs are very useful tools for firefighters in smoke-filled enclosures, although their performance could be improved combining thermal with other remote sensing techniques.

2.2. Underwater imaging systems

There is a very good review by P. Johnsson in [67] showing underwater acoustic and video-based methods. Armies all over the world have sponsored research and articles have been written identifying the key challenges for future development [68]. Challenging as it is, the topic of acoustic imaging is a very well established and mature research field, as is underwater video. These two fields that may seem unrelated become closely related when it comes to underwater deployment of imaging systems. A short discussion of their advantages and disadvantages will be given next.

2.2.1. Acoustic systems

Acoustic systems have been around for many years now: it is believed that Leonardo Da Vinci had already described a rudimentary passive SOUNd NAVigation and Ranging (SONAR) by 1490, and by 1925 the principles of the echo-sounder were firmly established. The main use of echosounders is measuring geometry,

³Dual use goods are products and technologies normally used for civilian purposes but which may have military applications. In Spain, RD2061/2008 [63] modified by RD844/2011 [64] and ECC/705/2013 [65], and more recently RD679/2014 [66] regulate external commerce of defense and dual-purpose products and technologies.

(a) Principle of operation of an echosounder. Taken from punaridge.org

(b) Multibeam echosounder with high resolution for the Institute of Oceanography – BAS, Varna. Courtesy of Lomini Ltd.

Fig. 2.7.: Echosounder: principles and real device.

usually bathymetry⁴, in the sea. Bathymetry is of importance in navigation as well as in topographic research and other areas such as search-and-rescue or military operations.

Acoustic systems have the advantage of being relatively immune to scattering at the frequencies of use, which means that changes in temperature of water, sediments or other small artifacts do not interfere with acoustic signals. This property is very advantageous since it opens the door to acoustic-based imaging systems (see [69, 70, 71] and other uses in [72, 73]), which is the idea behind many papers and some firms proposing acoustic cameras. Sound is used to produce a map of reflected intensities. These images often resemble optical images, and the level of detail can be very high. There are sophisticated commercial models available that show a high level of accuracy [74].

On the other hand, acoustic images cannot always be interpreted straightforward from the information displayed but by trained staff. In that sense, the response and brightness of the different pixels in the image depend on the angle of incidence, roughness of the surface, acoustic shadows and other artifacts as in the examples shown in Figure 2.8.

Regular echosounders result too big and power consuming to consider for a practical setup within the scope of this thesis (Figure 2.7(b) shows a real device): Handheld mobile devices are desired and therefore higher frequencies –in the MHz range– should be used. This comes at the cost of increased attenuation and therefore shorter operational range. The resulting range will depend on the power radiated and the features of the medium.

⁴From the Merriam-Webster Dictionary: “*Bathymetry*. the measurement of water depth at various places in a body of water; *also*: the information derived from such measurements”.

(a) Taken from [75]. Examples of new data collected in three different parts of Harrison Bay in August 2010.

(b) Side scan sonar image of the *Frank A. Palmer and Louise B. Crary*. Courtesy of NOAA/SBNMS and NURC-UConn.

Fig. 2.8.: Comparison between unprocessed and processed acoustic images.

2.2.2. Optical systems

The use of optical systems for underwater exploration comes from the natural evolution of surface photography and video. From Jacques Cousteau to ocean drilling or military operations, underwater video systems have evolved since they first appeared in the 1940's. Traditional approaches suffer from the same problems we are trying to address. To name a few:

- Visibility due to the **optical properties of water**: one of the most obvious properties of water is that the deeper the darker. This is due to the fact that the light from the sun is absorbed and scattered, forming what some have named "veiling light" [3]. Besides, absorption affects different frequencies in a different manner. Lower frequencies (red) tend to disappear first, while higher frequencies (blue) are the last ones to vanish. Hence the typical blue color of the oceans.

Several authors have pointed their research towards underwater image processing (see an example in Figure 2.9). It is possible to partially compensate for the loss of color and visibility using properties like the polarization of scattered light underwater [76, 77]. Others have studied the effect of external illumination of the scene using unstructured or structured (patterns, monochromatic, etc.) light. Techniques such as collimating the incident ray, gating⁵, etc. have also been used [78].

- **Turbidity**: changes in temperature may lead to changes in density and thus underwater currents which will affect the propagation of light.
- The existence of **sediments or other particles** suspended (microscopic al-

⁵Gating is a sensing technique that blocks all input to the sensor but from a certain distance range.

Fig. 2.9.: Raw image vs. “recovered” image using polarization techniques. The point in the recovered image part is twice as distant as the one in the raw image part, indicating the increase of visibility range (taken from [3]).

(a) Underwater oil infrastructure

(b) Ship wreck

(c) Boat

Fig. 2.10.: Examples of DIDSON camera images.

gae, krill and other plankton, etc.) affects the way light is scattered. Of utmost importance in caves and other confined spaces, a wrong movement done by a diver may mean the complete loss of sight in a matter of seconds. It may take hours or even days for sediment to settle once moved.

It is worth pointing out the use of laser in later years. Its inherent collimation and coherence has been viewed as an opportunity by many authors, who have conducted studies taking advantage of their imaging and ranging properties [79].

Jules S. Jaffe, in a 1990 paper [80] provides with an insightful description of a computer model explaining the formation of underwater images. The model incorporates intrinsic as well as apparent features of the propagation of light in water. It examines the performance of different lighting systems, both in-line and displaced. He concludes that huge gains in image contrast can be obtained by introducing carefully designed lighting and other techniques such as gating.

Finally, it is interesting to underline the good results obtained when combining the favorable properties of both acoustic and optical domains onto single devices.

Impressive results have been achieved in [81], combining propagation properties of acoustic waves –dual frequency identification sonar– and optical resolutions thanks to “sonar lenses” [82]. The concept of “sonar lenses” is very interesting, since it bridges the gap between optical and acoustic domains. The performance of these cameras can be seen in Figure 2.10.

Once the devices and systems used at the time of writing are presented, it is clear that a deep understanding of the physical processes inherent to signal propagation and its alterations is important to achieve a good understanding of the problem we are dealing with. Next chapter will dive into the foundations of remote sensing.

3. Remote sensing for location awareness. Foundations

"We know from science that nothing in the universe exists as an isolated or independent entity."

Margaret J. Wheatley

This chapter explores the most relevant approaches to artificial vision that may be of interest for user location awareness in harsh environments. Features of both *mechanical and electromagnetic domains* will be studied. Basic properties of acoustical and optical radiation will be compared, underlining their similarities and differences: the aim is to provide the reader with an overview of the underlying physics and what can be expected from each type of wave when they face a certain scattering medium.

Mechanical and electromagnetic domains share concepts from a system's point of view. The underlying principle is simple: the idea is to measure the time a certain wave spends traveling from the emitter to an obstacle, interact with it, and return to the receiver. The time measured can be converted to distance taking into account the propagation properties of the ongoing/returning wave and its interactions with the medium through which the wave has been propagated. If this process is repeated with enough resolution and speed it may be possible to build an image of the environment.

The idea of building from scratch a novel approach to the systems and devices used today in harsh environments is complex and rises many questions. In general, a remote sensing device is made up of several subsystems (see Figure 3.1):

1. **Sensing Element:** Be it piezoelectric, optical or an antenna, this element is the heart of the device and the most difficult element to design. It will have to address the medium and its constraints (dispersion, attenuation, etc.). Its performance will determine the maximum resolution of the final device and its ultimate performance. It will be a challenge to design and build.
2. **Data Acquisition Unit:** It is responsible for handling the raw data coming from the sensing element into a suitable form for further processing. Its design will have to take into account the trade-off between speed and ac-

Fig. 3.1.: Concept and overview of a remote sensing system.

curacy, not to forget memory and overall power consumption (for instance, adaptation to embedded platforms).

3. **Signal Processing Unit:** This module will process the data as presented by the Data Acquisition Unit. Implementation of new algorithms or adaptation of existent ones in Digital Signal Processors (DSPs) or Field-programmable Gate Arrays (FPGAs) will be done in this module (border detection, image handling and filtering etc.).
4. **Other Signal Processing Units:** They will be in charge of the extraction of data from other subsystems, such as thermal imagers, pressure sensors, etc. in order to integrate it with the data from the Sensing Element.
5. **Presentation Unit:** It will integrate the data from the different subsystems and present it to the user.

As a starting point, mechanical (acoustics) and electromagnetic (optical) signals will be analyzed in next sections, underlining the key figures that have to be taken into account in order to make design decisions. After a general introduction on the types of signals, several aspects of each approach will be examined: generation –which will cover the techniques available in order to create the desired signal–, propagation –where the relevant distortion mechanisms will be identified–, data acquisition and limitations –pointing to state of the art limitations in aspects such as speed, resolution, etc.– and technology. Other options such as terahertz, metamaterials, etc. and their prospective potential in remote sensing will be discussed last.

3.1. Acoustics

Acoustic signals consist in the propagation of pressure waves. Mechanical waves as they are, their velocity can be expressed in terms of their *bulk modulus*: the ratio of the change in pressure to the fractional volume compression is called the bulk modulus of the material, $B = \frac{\Delta P}{\Delta V/V}$, where P is pressure and V volume. Besides,

the velocity v of a mechanical wave can be expressed as

$$v = \sqrt{\frac{\text{elastic property}}{\text{inertial property}}} = \sqrt{\frac{B}{\rho}} \quad (3.1)$$

where B is the bulk modulus and ρ the density of the medium. In gases, the velocity of sound is given by

$$v_{\text{sound}} = \sqrt{\frac{\gamma RT}{M}} \quad (3.2)$$

where γ is the adiabatic constant of the gas (1.4 for air), R is the universal gas constant (8.31JK/mol), T is the temperature in Kelvin and M is the molecular mass of the gas in grams. In air, the velocity of sound is given by (taking $M = 28.9\text{g/mol}$ and substituting in the previous equation):

$$v_{\text{sound, air}} = 20.05\sqrt{T}[\text{m/s}] \quad (3.3)$$

which yields velocities in the range of 340m/s at room temperatures and 540m/s at fire temperatures (450°C). In water, propagation ranges from 1450 to 1550m/s depending on salinity, temperature, etc.

In general, waves are characterized by their intensity, frequency f and pulse shape.

$$f = \frac{v}{\lambda} \quad (3.4)$$

where λ is the wavelength and v the propagation speed. Equation 3.4 is valid for all sorts of waves.

Frequency and thus wavelengths determine in general the maximum resolvable feature (see Table 3.1). It is therefore important to choose an appropriate frequency for the application intended.

Another important feature is pulse shape and length. Different pulses (see Figure 3.2) have also different detection properties and processing complexity [83, 84]. The duration of a signal burst (train of pulses) impacts directly on the resolution: two pulses of duration T can only be distinguished if separated by a time of at least T , which yields a spatial resolution of $vT/2$ (for a 1ms pulse and typical values for v , 0.75m in water or 0.17m in air at 300K).

Waveforms have also implications on the overall system performance: chirps (FM sweeps) are more difficult to process but give better results under heavy noise conditions. Gaussian pulse derivatives are becoming more used as signal processing power increases: they have maximum steepness of transition with no overshoot and minimum group delay at the cost of higher computational load. These facts apply to electromagnetic waves as well.

Acoustic waves have been widely used in mapping the seabed, in depths ranging from a few centimeters to several kilometers. Acoustic echoes provide with

Tab. 3.1.: Maximum resolvable feature as a function of wavelength λ .

Medium	Sound Speed (m/s)	Frequency (kHz)	Wavelength (λ , in mm)
Water	1500	1	1500
		5	300
		10	150
		20	70
		50	30
		100	15
		200	7
		500	3
		1000	1.5
Air @300K (26.85°C)	347.3	1	347.3
		5	69.46
		10	34.73
		20	17.36
		50	6.95
		100	3.47
		200	1.74
		500	0.69
		1000	0.34
Air @723.15K (450°C)	539.2	1	539.2
		5	107.84
		10	53.92
		20	26.96
		50	10.78
		100	5.39
		200	2.69
		500	1.08
		1000	0.54

Fig. 3.2.: Examples of Chirps, Continuous Wave (CW) pulses and Bursts.

information about distance and composition of the seabed. SONAR can provide accuracies up to a few centimeters (see [85] for a comprehensive text on SONARs).

3.1.1. Generation

Acoustic waves are produced by vibration of a physical medium (air, water, other fluids and solids). For underwater use, the electro-acoustical transducers employed are called hydrophones and consist of arrays of several piezoelectric elements made of ceramic materials that are of choice for the frequencies implied. The design parameters of the hydrophones resemble those of RF antennas (gain, beam collimation, etc.).

Parameters such as 3dB bandwidth, directivity and relative bandwidth of the individual elements of the array determine the imaging properties of the device. Hydrophones part of a sonar tend to have very high directivities in the along track direction (usually a fraction of a degree) and very low directivities in the across track direction (about 40-60°). Excitation signals have to be carefully chosen in order to minimize undesired effects such as ringing, resonations and mixing of successive echoes. There are many texts covering the topic of antenna theory and design (see [86] to cite one). While most of them are devoted to RF, the basic principles hold for acoustic waves.

Improvements in directivity patterns have been achieved in recent times using arrays with spatial adaptive signal processing (*beamforming*) [87, 88]. The basic principle behind beamforming is that it is possible to mimic high directivity antennas by introducing adequate delays in the signal transmitted by each element of the transmitter –the same is valid for reception–. Simpler beamformers have the drawback, however, that a detailed knowledge of the characteristics of the operation noise is required to use them, which is difficult in practice and can lead to malfunction of the adaptive algorithm. Beamforming and Synthetic Aperture make it possible to achieve controllable directivities at the cost of higher system complexity, opening the door to high resolution scanning systems.

More sophisticated algorithms include means of detecting sources of interferences and other distortions in real time. This way, the adaptive algorithms will place zeroes in the directions where perturbations come from [89]. This theory can be generalized from 1D arrays to other 2D and 3D beamformers.

3.1.2. Propagation

Mechanical waves are affected during their trip from the emitter to the target and all the way back to the receiver manifold:

- In the far field (see Table 3.2) they behave as planar waves, their intensity reducing as a factor of $1/R^2$, R being the distance from the emitter. That

Tab. 3.2.: Radiation zones as a function of λ .

Zone	Range
Near-field (non-radiative)	$< \lambda/3$
Near-field (radiative or Fresnel zone)	$(\lambda, \frac{L^2}{4\lambda})$, L the emitter size
Far-field (Fraunhofer zone)	$\geq \frac{L^2}{4\lambda}$

Fig. 3.3.: Effect of refraction on range misestimation.

reduction in energy and therefore intensity is called **attenuation**. Other factors contributing to the attenuation of the wave are due to interactions with the medium, such as absorption of energy.

- Acoustic waves also follow Descartes-Snell law of **reflection and refraction** at interfaces (equation 3.5; n_i are the indices of refraction and θ_i the incident and refracted angles).

$$n_1 \sin \theta_1 = n_2 \sin \theta_2 \quad (3.5)$$

Two layers of air or water at different temperatures will have different refraction indices and will therefore deviate the wavefront. This fact can have a direct effect on range measurements (see Figure 3.3).

- Another important effect is **acoustic scattering**. It is determined by the angle of incidence of the incoming acoustic wave with the object under study or, more generally, with any objects or particles encountered along path. When reaching an object, some of the energy will be reflected in the specular direction (following the *law of reflection*). The rest of the incident energy will be absorbed by the object or reflected in other directions (scattered); even some of the remaining energy will scatter back in the incoming direction (*backscatter*). Backscattered radiation is usually several orders of magnitude lower than the emitted radiation.

The backscattered energy reaching the receiver will provide different types of information. The time of flight will give the *slant range* (distance between

the emitter and the object) if exact knowledge is provided for the velocity of the sound in each and every point traveled by the acoustic wave. Frequency and phase shifts are used to determine the relative speeds of the sensor and the object and the arrival angle of the wave. Other properties of the objects can be retrieved as well [90]. The measurement and characterization of those interactions can be of use to identify the object encountered by the incident wave or its properties.

Backscattering is affected by

- the **relative angle** of the incident wave with the target, and
- the **physical properties** of the target, both macroscopic (flatness/roughness)¹ and microscopic (interaction between the incident wave and the molecules upon which the object is formed).

Smooth surfaces (important: *at the scale of the incident wavelength*) will give more specular radiation and less backscatter when compared with rough surfaces at that same scale. Wavelength is important because surfaces appearing flat at some wavelengths may appear rough at others. Another important factor is the relative angle of incidence: for the same constituent material, a surface facing the incident radiation will have higher backscattering than a surface parallel to the incoming radiation. Although not considered here, the interactions between the incident acoustic wave and the particular target material will determine the amount of energy refracted and absorbed. Underestimation of these factors can lead to misinterpretation of artifacts that will surely appear as a result of the combined effect of the aforementioned phenomena.

There are many models to simulate scattering at surfaces, but the simplest one is Lambert's cosine law, which approximates backscatter to the square cosine of the incident radiation [92]. The qualitative effects of surface roughness and relative angle of incidence are depicted in Figure 3.4.

In general, it is possible to say that scattering depends primarily upon the size of the scatterer² (D) and the incident wavelength (λ). Three main types of scattering have been studied accordingly [93, 94]: Rayleigh scattering ($\lambda \gg \pi D$), Mie scattering ($\lambda \approx \pi D$) and Geometric scattering ($\lambda \ll \pi D$).

Many more models for scattering have been developed because of its military potential –scattering can be used to identify the object being radiated–. When it comes to the scope of this thesis (professional working conditions for humans), for acoustic waves Geometric and in some cases Mie scattering

¹Features of size comparable to the wavelength of the incident acoustic wave. Following the Rayleigh criterion, a surface is considered smooth if $d < \lambda/(8 \cos \theta)$, d being the height of surface irregularities [91].

²In the case of complex geometries, D must be a “representative” size, taking into account λ and the cross section of the scatterer.

Fig. 3.4.: Effect of surface roughness ((a) vs. (b)) and surface tilt ((c) vs. (d)) on reflection, scattering and backscatter.

will be predominant for air atmospheres with suspended particles, while Rayleigh and in some cases Mie scattering will be predominant for water atmospheres with suspended particles. The basic principles of scattering are common to electromagnetic waves.

The radiation zone where the interaction takes place is also relevant. Acoustic waves emanating from a emitter contain evanescent fields, which decay rapidly with distance. The zone where those fields have observable effects is called *non-radiative near-field zone*. There is then an intermediate zone where radiative and non-radiative fields can coexist (*radiative near-field zone* or *Fresnel zone*) and last the radiation zone, also known as *far-field region* or *Fraunhofer zone* (see Table 3.2).

The preferred zone of operation for remote sensing applications is the far-field region as it is where the emitted radiation behaves as a planar wave –there the angular field distribution is independent of the distance to the emitter–. However, near-field operation and the evanescent fields associated with it (detectable in the first $\lambda/3$ region from the emitter) are attracting more and more attention from physicists as they have interesting properties such as *superresolution*: evanescent waves are not constrained by diffraction resolution limits ($\approx \lambda/2$, the Abbe limit that otherwise applies to propagating waves³).

Considering search-and-rescue operations or technical diving, meter ranges would be normal. The exact application would therefore condition a range of valid wavelengths to ensure far-field operation ($> 2D^2/\lambda$ in the case of electrically large antennas) with a resolution $\approx \lambda/2$ in the best case .

3.1.3. Data acquisition and limitations

The detection process can be regarded as the inverse of the emission process. In that sense, acoustic receivers, hydrophones or microphones (depending on whether they work under water or in air) are characterized by directivity patterns, detection limits and noise figures –among other parameters–. They can be either narrowband or broadband detectors. Narrowband detectors are sensitive to relative motion between the emitter and the target: the Doppler effect can lead to changes in frequency that can move the incoming acoustic signal out of the reception band. On the other hand, broadband detectors are more suited for moving targets but also gather more noise. The *Figure of Merit (FOM)* is the basic performance measure for SONARs [89]:

$$\text{FOM}_{\text{active}} = L_S + N_{\text{TS}} - (L_N - N_{\text{DI}}) - N_{\text{RD}} \quad (3.6)$$

where

³Abbe was the first one to define the term Numerical Aperture. He has been credited with the derivation of the diffraction limit [95] although it is believed that Joseph L. Lagrange was actually the first one to derive it.

L_S	Source level
L_N	Noise level
N_{DI}	Directivity index
N_{TS}	Echo level or target strength
N_{RD}	Recognition differential

FOM is a means of comparing different SONARs: a bigger FOM means better reception capabilities. It is obvious that comparing different systems for a particular application involves many more parameters and a richer study of their performance.

The directivity patterns of the receivers should at least match the directivity patterns of the emitters, so that they receive input from all the points illuminated and the least possible from the points not directly illuminated. This holds for electromagnetic systems as well. In many SONAR systems, the same device acts as emitter and receiver.

SONAR imagery, like any other data, is not free from defects or artifacts. Proper processing of the raw data plus extensive training of users can lead to its minimization within the operation framework. Even if it is not possible to prevent artifacts from occurring it is possible to maximize their detection and action can be taken in order to minimize their effects. In artificial vision systems, a system able to filter out or discriminate those artifacts is highly desirable.

In general, footprint size –product of the across track resolution Δx times the along track resolution Δy – will determine the maximum theoretical resolution achievable. Acoustic beams spread with growing distance from the source and therefore resolution decreases yielding way to fainter returns from targets.

Another important parameter is the maximum achievable range, which will be directly influenced by propagation constraints of the selected waveform and frequency in the particular medium (air, water, smoke,...). The maximum range will be limited by background noise, scattering, multipath and the detector properties, taking into account that for artificial vision systems ranges can be limited to tens of meters, specially for confined spaces or heavy particle-filled atmospheres. The received signal will be equal to the convolution of the signal sent with the angular transmission pattern of the medium.

Physical constraints aside, it is possible to enhance detection of the origin of the returning echo with **advanced signal processing techniques** [89] including recursive filters (adaptive systems such as Wiener or Kalman filters) and interferometry. From the simplest techniques that include complete coverage of the area (superposition of the emitted beams) to other more advanced such as synthetic aperture processing, several techniques have been used, for instance in music for source localization [96] or crack identification [97]. There is active research ongoing in this area.

Sometimes, it is possible to treat propagation of acoustic waves as ray-tracing [98,

99] if the depth-to-wavelength ratio κ is very high (> 100 , only valid for very high frequencies –ultrasounds when dealing with artificial vision systems–):

$$\kappa = \frac{\text{depth}}{\lambda} > 100 \quad (3.7)$$

In addition, as stated in section 1.2, SONAR and echolocation [40] scientists study natural structures (for instance, jaws in dolphins [42], ears in bats [100], etc.). Further understanding of those structures can help gain knowledge that may be useful in creating the next generation of sound-based imaging devices.

3.1.4. Technology

Electroacoustic transducers are the elements that convert electrical signals into acoustic signals (also called projectors) and *vice versa*. These transducers are reciprocal devices, in the sense that projectors can act as hydrophones and the other way round. Due to their chemical constitution and, more specifically to their lattice, they accumulate electrical charges in a certain region of their internal structure when subjected to mechanical stress, and in the opposite region of the lattice when the mechanical stress comes in the opposite direction [101].

Hence, vibrations cause the alternative accumulation of electrical charges in one or another zone of the material proportional to the mechanical stress in the lattice. There are many natural and also engineered piezoelectric materials, but some of the most used are the family of ceramics with perovskite or tungsten-bronze structures [102]. An example of the former type would be lead zirconate titanate ($\text{Pb}[\text{Zr}_x\text{Ti}_{1-x}]\text{O}_3$, $0 \leq x \leq 1$), more commonly known as Lead Zirconate Titanate (PZT), which is the most common piezoelectric ceramic in use today.

3.2. EM: Optics

Electromagnetic waves share most of the physical behavior and concepts shown for acoustical waves. In addition, they have been subject of extensive research during the XX century yielding many applications, also in imaging [103]. For the artificial vision applications in the professional environments subject of this thesis it is desirable to use highly collimated beams and, wherever possible, aim for mobile solutions. This is the reason why electromagnetic signals at optical frequencies (treated as higher RF frequencies) will be preferred and thus the subject of a more in-depth analysis.

3.2.1. Generation

Optical remote sensing will be taken almost as a synonym for Light Amplification by Stimulated Emission of Radiation (LASER) remote sensing due to the capabilities of its coherent emission of light, centering the discussion on the performance and applicability of LASER⁴ for practical cases. Its highly collimated beam and availability makes it perfect for remote sensing applications.

Due to recent advances in solid state physics, it is possible to have lasers emitting in many different wavelengths, from visible to infrared and UV [4]. This availability over a high range of frequencies extends the advantages of solid-state devices (integration, reproducibility, controllability,...) to many applications, alone or combined with other technologies [104]. Figure 3.5 shows the availability of different types of lasers as a function of their operating frequency.

Regardless of the specific radiation mechanism, the laser will be considered as a source of highly collimated, practically monochromatic radiation, which may be continuous or pulsed (see [105] for a discussion on potential capabilities of both kind of lidars). Assuming high beam collimation and no scattering, the one-dimension **radiative-transfer equation** can be written as:

$$\frac{dJ(\nu, z)}{dz} = \epsilon(\nu, z) - \kappa(\nu, z)J(\nu, z) \quad (3.8)$$

where ν is the frequency considered, z is the direction of propagation, $\epsilon(\nu, z)$ is the *volume emission coefficient* per steradian (see [106] for details) and $\kappa(\nu, z)$ is the *volume absorption coefficient*. $J(\nu, z)$ is the *spectral radiance*.

Defining the *source function* as

$$S(\nu, z) \equiv \frac{\epsilon(\nu, z)}{\kappa(\nu, z)} \quad (3.9)$$

and the *optical depth* τ corresponding to a path of length l

$$\tau(\nu, z) = \int_0^l \kappa(\nu, z) dz \longrightarrow d\tau(\nu, z) = \kappa(\nu, z) dz \quad (3.10)$$

Solving the equation for the spectral radiance at $z = l$, $J(\nu, l)$:

$$J(\nu, l) = J(\nu, 0)e^{-\tau(\nu, l)} + e^{-\tau(\nu, l)} \int_{\tau(\nu, 0)}^{\tau(\nu, l)} S(\nu, z)e^{\tau(\nu, z)} d\tau(\nu, z) \quad (3.11)$$

If the medium is homogeneous,

$$\tau(\nu, l) = \kappa(\nu)l \quad (3.12)$$

⁴From now on, laser will be written in lowercase: it can be considered to have entered the language as an everyday word.

Fig. 3.5.: Commercial LASERs and their operating wavelengths. Picture by Danh [CC BY-SA 3.0], compiled using data from [4].

and then

$$J(\nu, l) = J(\nu, 0)e^{-\kappa(\nu)l} + S(\nu)[1 - e^{-\kappa(\nu)l}] \quad (3.13)$$

$S(\nu)$ is zero for “cold” (non-excited) mediums since $\epsilon(\nu)$ will be zero. If $\kappa l \ll 1$ the medium is said to be *optically thin*. Else, the medium is said to be *thick*. Therefore, for cold mediums,

$$J(\nu, l) = J(\nu, 0)e^{-\kappa(\nu)l} \quad (3.14)$$

If scattering is considered along absorption, the radiative-transfer equation becomes much more complicated. It is possible to introduce the *total attenuation coefficient*

$$\kappa_e = \beta_A(\nu) + \beta_s(\nu) \quad (3.15)$$

where $\beta_A(\nu)$ and $\beta_s(\nu)$ are the absorption and scattering coefficients respectively. For a well-confined beam propagating in the z direction, the steady-state radiative-transfer equation, with scattering, takes a complicated form that is reproduced below only for illustrative purposes:

$$\frac{dI(\nu)}{dz} = \epsilon(\nu)\Delta\Omega - \kappa_e(\nu)I(\nu) + \int_{\Delta\Omega} d\Omega \int_0^\infty d\nu^* \int_{4\pi} d\Omega^* \beta_s(\nu^*, k^* : \nu, k) J(\nu^*, k^*) \frac{\nu}{\nu^*} \quad (3.16)$$

The first term in the right hand side of the equation accounts for the volume emission, the second for the attenuation, the third for the scattering and I can be expressed as

$$I(\nu) \equiv \int_{\Delta\Omega} J(\nu, k) d\Omega = c\Delta\rho(\nu) \quad (3.17)$$

This general equation can be reduced under clear conditions to a simple exponential decay.

3.2.2. Propagation

As in the previous case with acoustic waves, electromagnetic waves can be described as wavefronts propagating through space. This involves a field representation of the wave, which is consistent and directly related to Maxwell's equations [107]. Another approach is called *geometric optics*, which studies the direction of propagation of the wave and its interaction with the medium, modelling the wave as a ray (raytracing). This approach will be used in the development of the propagation model presented in chapter 5.

Unlike representations of mechanical waves, which produce material displacements or changes in a certain physical magnitude (e.g. pressure) due to the propagation of a mechanical wave, electromagnetic waves do not move matter: they provoke changes in the magnitude of electrical and/or magnetic fields (see Figure 3.6). Electromagnetic waves can be also treated as plane waves if seen at a certain distance from the antenna (far-field) [108].

Fig. 3.6.: Electromagnetic & acoustic waves: Waveforms and their physical treatment.

The basic reason is that Maxwell's equations prescribe different behaviors for each of the two source terms of electric fields and also the two source terms for magnetic fields, which account for changes in the performance of electromagnetic fields with distance from their source. Common derivations solve Maxwell's equations for a short radiating wire (dipole) and analyze the solution [109]. Several conclusions can then be derived:

- There is one inverse distance term –proportional to $(\frac{1}{r})$ –, which is called the radiation term. This term represents the flow of energy away from the wire.
- There is also one inverse square distance term –proportional to $(\frac{1}{r^2})$ –, which is called the induction term and represents energy stored in the field during one quarter of a cycle and then returned to the antenna in the next one.
- And finally there is one inverse cube distance term –proportional to $(\frac{1}{r^3})$ –, called the quasi stationary term, or the electrostatic field term, and results from the accumulation of charge at the ends of the element.

The contribution of the radiating term is bigger than the induction and the electrostatic terms at distances longer than $\lambda/2\pi$, which is the distance appointed by some as the near-field limit. These dipole near-field intensities may be very powerful near the source but decay very rapidly with distance in comparison to the radiation term (the far-field). At distances farther than $\lambda/2\pi$ they still exist and can be significant in a region known as transition zone.

Both near-field and transition regions are subject to decision of what can be understood by “significant” contribution to total fields, which is the reason why the

Tab. 3.3.: Near-field thresholds for different cases. Adapted from [14].

Definition	Remarks
$\lambda/2\pi$	$1/r$ term is dominant
3λ	D (antenna diameter) not $\gg \lambda$
$\lambda/16$	Measurement error $< 0.1\text{dB}$
$\lambda/8$	Measurement error $< 0.3\text{dB}$
$\lambda/4$	Measurement error $< 1\text{dB}$
$\lambda/2\pi$	Satisfies the Rayleigh criteria
$\lambda/2\pi$	For antennas with $D \ll \lambda$ and printed-wiring-board traces
$2D^2/\lambda$	For antennas with $D \gg \lambda$
$4D^2/\lambda$	For high-accuracy antennas
$50D^2/\lambda$	For high-accuracy antennas
$3\lambda/16$	For dipoles

limits of the regions have been placed in different points (read [14] for a clarifying paper on near- vs. far-field criteria). For remote sensing applications within the framework of this thesis, Transverse Electric and Magnetic (TEM) waves and thus clear far-field operation will be of choice, in agreement with [14] and the values given in Table 3.3 for the different cases.

As in the acoustics section, several important aspects of electromagnetic signal propagation will be discussed below:

- **Polarization** is a property of waves that can oscillate with more than one orientation. It is a remarkable difference between acoustic and electromagnetic signals, because longitudinal mechanical waves (and as such, acoustic waves in gases or liquids) can only vibrate in the direction of propagation. Polarization affects the design of transmitters and receivers since the orientation of the antenna determines the polarization of the emitted wave (elliptic, circular or linear). In that sense, the detected field E_d is proportional to the dot product of the polarization vectors of the antenna $\vec{P}$ and the incident wave $\vec{E}_i$:

$$E_d \propto \vec{P} \cdot \vec{E}_i \quad (3.18)$$

Polarization may change when interacting with materials. It is an important factor to take into account because changes in polarization can be related to the particular material that interacts with the incident signal: this can be used in remote sensing to gather knowledge about the material returning the echo. State of the art defense equipment makes use of this property to gain insight from particular targets. However, it may lead to unexpected drops in signal reception caused by the dot product of the antenna and the undesired polarized echo. Given the target applications considered, robustness will be favored. Polarization is in any case a matter of careful deci-

Fig. 3.7.: Scattering regimes for single scattering by spheres and different particle size parameters. Taken from [5].

sion since it depends on the signal propagation path for the frequencies involved [110]. The interested reader is pointed to any book covering the electromagnetic theory in depth.

- For the limited range of operation needed for temporary loss of vision applications, both EM **absorption and attenuation** will not be the killer conditions of the system since the propagation path in free space will be usually in the meter range and well under 100m roundtrip –a visual range of tens of meters will normally suffice–.
- An important subject in optical remote sensing is **scattering**. The basis and fundamental explanation is the same as for acoustic waves, although the relative particle sizes in the medium considered compared to the incident wavelength will be different and thus the dominant scattering type and its effects will vary. Figure 3.7 shows the different types of scattering as a function of particle size and wavelength. The relative importance of scattering for optical remote sensing suggests conducting an in-depth analysis due to its weight in the final performance of an artificial vision system.

The first relevant scattering mechanism in optical remote sensing is *molecular Rayleigh scattering*, which is the elastic scattering of light or other electromagnetic radiation by particles much smaller than the wavelength of the incident light such as individual atoms or molecules. A good reference on

scattering is the text by Measures [106]:

$$\frac{dP(\theta, \phi)}{d\Omega} = \frac{1}{2} \epsilon_0 c |E_0|^2 r_e^2 \left[\frac{\omega^2}{\omega_0^2 - \omega^2 - j\omega\gamma} \right]^2 \{\cos^2 \phi \cos^2 \theta + \sin^2 \phi\} \quad (3.19)$$

where P is the power radiated in spherical coordinates, ϵ_0 the dielectric constant of the medium, c the velocity of light, E_0 the incident electric field, r_e the distance of the point considered to the particle, ω is the wavenumber of the incident radiation, ω_0 is related to the induced acceleration of the bound electron, and the rest of the terms are related to the position of the point considered.

Defining the differential scattering cross section of a molecule or atom as $d\sigma/d\Omega$ it is possible to write that

$$\frac{dP(\theta, \phi)}{d\Omega} = I_0 \frac{d\sigma(\theta, \phi)}{d\Omega} \quad (3.20)$$

where

$$I_0 = \frac{1}{2} \epsilon_0 c |E_0|^2 r_e^2 \quad (3.21)$$

r_e being the classical electron radius and

$$\frac{d\sigma(\theta, \phi)}{d\Omega} = \left[\frac{\omega^2}{\omega_0^2 - \omega^2 - j\omega\gamma} \right]^2 \{\cos^2 \phi \cos^2 \theta + \sin^2 \phi\} \quad (3.22)$$

At optical frequencies $\omega \approx \omega_0$ so

$$\frac{d\sigma(\theta, \phi)}{d\Omega} \approx \frac{1}{4} r_e^2 \{\cos^2 \phi \cos^2 \theta + \sin^2 \phi\} \left[\frac{\omega^2}{(\omega_0 - \omega)^2 + (\gamma/2)^2} \right] \quad (3.23)$$

Integrating σ :

$$\sigma_R(\omega) = \frac{2\pi r_e^2}{3} \left[\frac{\omega^2}{(\omega_0 - \omega)^2 + (\gamma/2)^2} \right] \quad (3.24)$$

In terms of the complex refractive index of the medium n and $\lambda = 2\pi c/\omega$:

$$n^2 = 1 + \frac{Ne^2}{\epsilon_0 m_e} \left[\frac{1}{\omega_0^2 - \omega^2 - j\omega\gamma} \right] \quad (3.25)$$

where N is the atom density of the medium, e the electron charge and m_e the electron mass.

The total backscattering cross section $\sigma_R(\lambda)$ can be evaluated integrating over 4π steradians:

$$\sigma_R(\lambda) = \frac{8\pi}{3} \left[\frac{\pi^2 (n^2 - 1)^2}{N^2 - \lambda^4} \right] \quad (3.26)$$

The *backscattering cross section* is of vital importance in optical remote sensing and takes the following form:

$$\sigma_{\pi}^R \equiv \frac{d\sigma_R(\theta = \pi)}{d\Omega} = \frac{\pi^2(n^2 - 1)^2}{N^2\lambda^4} \quad (3.27)$$

The other important scattering mechanism that will affect optical remote sensing is the *Rayleigh-Mie scattering*. For instance, air can consist of a number of aerosols comprising dust, soot, ash, fogs, haze, etc. and water of others such as microplankton, mud, etc. whose sizes span over several orders of magnitude [111]. Their scattering properties become extremely complex when their dimensions come to be comparable to the wavelength of the incident radiation.

Hence, it is convenient to define the *scattering size parameter*:

$$\alpha = \frac{2\pi a}{\lambda} \quad (3.28)$$

where a is a representative size of the particle in suspension. For isotropic dielectric scatterers whose size is much smaller than the wavelength illuminating them ($\alpha < 0.5$ or $a < \lambda/4\pi$) the scattering can be approximated to molecular Rayleigh scattering. If the scatterer is modelled after a sphere of radius a and refractive index n it is possible to express the backscattering cross section for the isotropic dielectric sphere as:

$$\sigma_{\pi}^R \equiv \frac{d\sigma_R(\theta = \pi)}{d\Omega} = a^2(ka^4) \left\{ \frac{n^2 - 1}{n^2 + 2} \right\}^2 \quad (3.29)$$

which has the same λ^{-4} and angular dependence of the molecular Rayleigh scattering.

For electrically bigger scatterers ($\alpha > 0.5$) the scattering becomes depending on the angle. This is why large scatterers scatter all wavelengths equally in all directions and thus tend to appear white (e.g. clouds). The first study of scattering of light in particles with sizes comparable to that of the scatterer was undertaken by Mie back in 1908 [112]. This theory states that in general for values of α over 0.5 the backscattering loses its symmetry and the differential scattering cross section becomes dependent on α , n and θ , with a pronounced *forward scattering* for values greater than 1.5 (see Figures 3.8 and 3.9). For cases where $ka \ll 1$ Mie scattering becomes similar to Rayleigh scattering.

There are two further scattering parameters that are of prime importance in the field which are included here for completeness, the *volume backscattering coefficient* β_{π} and the *total volume scattering coefficient* β_s . Following

Fig. 3.8.: Mie Scattering for different values of α : 0.2 (a-b), 0.5 (c-d), 1.5 (e-f) and 6.0 (g-h). Graph includes polar *linear* (a, c, e, f) plots, and the relative angle between incident and scattered radiation (b, d, f, h). Graphs show unpolarized (natural) radiation [red], parallel [i_2 blue], and perpendicular [i_1 green] scattering

Fig. 3.9.: Mie Scattering for different values of α : 0.2 (a-b), 0.5 (c-d), 1.5 (e-f) and 6.0 (g-h). Graph includes polar *log* (a, c, e, f) plots, and the relative angle between incident and scattered radiation, also in log scale (b, d, f, h) plots. Graphs show unpolarized (natural) radiation [red], parallel [i_2 blue], and perpendicular [i_1 green] scattering

the derivation in [106] we obtain a differential volume scattering coefficient equal to

$$\beta_j(\theta, n, \lambda) \equiv \frac{1}{2k^3} \int_{\alpha_1}^{\alpha_2} i_j(\theta, \alpha, n, \lambda) N(\alpha) d\alpha, \quad (j = 1, 2) \quad (3.30)$$

where i_j are the Mie intensity functions and α the size parameter.

Integrating gives the *total volume scattering coefficient*:

$$\beta_s(n, \lambda) \equiv \frac{\pi}{k^3} \int \alpha^2 Q_s(\alpha, n, \lambda) N(\alpha) d\alpha \quad (3.31)$$

where Q_s is the total scattering efficiency. The “*phase function*” –actually not representing anything related to the phase of the wave, but the angular radiation scattered by the medium– is:

$$P_j(\theta, n, \lambda) = 4\pi \frac{\beta_j(\theta, n, \lambda)}{\beta_s(n, \lambda)} \quad (3.32)$$

where $j = 1, 2$. β_j represents the *backscattering volume coefficient*. The *backscattering phase functions* are

$$P_j(\pi, n, \lambda) = 4\pi \frac{\beta_j(\pi, n, \lambda)}{\beta_s(n, \lambda)}, \quad (j = 1, 2) \quad (3.33)$$

When depolarization is negligible only β_π is considered.

There are computer programs that compute the contributions to the resulting Mie scattering, such as [113]. However, this analysis is restricted *strictu sensu* to sphere-like particles. A generalization of Mie theory to non-spherical particles has been undertaken by Barber and Yeh [114].

In real-world conditions it is important to consider *multiple-scattering*, which is dominant in environments with high turbidity (like in the particle-filled atmospheres). Multiple-scattering requires a more complex analysis, often involving statistical methods like the ones presented in [115, 116].

The scattering is said to be elastic if there is no change in wavelength after the wave-particle interaction has taken place, and inelastic (*Raman scattering*) otherwise. Raman scattering is not so relevant for artificial vision systems because it is about three orders of magnitude smaller than Rayleigh scattering. In pure water, scattering at optical frequencies is not so important because of the relative sizes wavelength-particle considered.

There is programming code and propagation models available in the internet addressing this problem [117, 55], most of them making use of numerical and statistical methods [118]. However, the majority has been designed for long distance applications (communications or atmosphere remote sensing) and hence they can be of limited use in this thesis. Others

have measured the optical properties of smoke plumes [119, 120, 121] or generated computer models for radiation computation in combustion environments [122]. Some authors have even questioned how those measurements were made [123]. Fortunately, despite the extraordinary complexity of scattering patterns and scatterers in the atmosphere the situation may be simplified when one of the mechanisms prevails.

3.2.2.1. Transmission properties of the atmosphere

The transmission properties of the atmosphere to electromagnetic radiation in particle-filled atmospheres is of utmost importance to assess the viability of a remote sensing system. In this section, the properties will be studied both at optical and other frequencies.

There has been extensive civil and military research [124, 125, 126] with the aim of characterizing air atmospheres for electromagnetic waves at microwave and millimeter frequency ranges. Atmosphere models have been created [6]; they are important in telecommunications, physics and other fields. Using the models it is possible to predict the behavior of the atmosphere for certain conditions. In Figure 3.10 the simulated zenith atmospheric transmission in the summit of the Mauna Kea volcano in Hawaii has been depicted as an example for two different precipitable water vapor values. Although the conditions shown in the figure are not directly extrapolatable to a fire scene in terms of temperature, obscurants and presence of chemicals that may affect propagation, the figure illustrates how relevant it is to know the composition and therefore, the properties of the medium at the frequency of choice in order to decide the best frequency to use. In that sense, it is important to underline the presence of absorption windows in the vicinity of 60 and 120GHz respectively, as well as the growing relevance of Precipitable Water Vapor (PWV) over 200GHz (40% absorption at 300GHz).

Other research has focused on specific conditions that may affect wave propagation of electromagnetic waves. One of such studies is the one conducted by Van de Wal [125], which discusses the effect of smokes and other man-made obscurants in the atmosphere. Another one [127] models the propagation of ice and suspended air/water particles for frequencies under 1THz. Independently of the accuracy and purpose of the different propagation models studied, it is possible to extract some basic conclusions for the propagation of electromagnetic waves in the atmosphere:

1. In the range of centimeter wavelengths (1m to 1cm, or 300MHz to 30GHz) the atmosphere is almost transparent, exhibiting only slight absorption of the radiation at frequencies in the upper range of the band (25-30GHz). This is due to the fact that the wavelengths considered are big compared to molecular sizes and thus are far away from natural resonating frequencies of the molecules found in the atmosphere. See Figure 3.10.

Fig. 3.10.: Simulated zenith atmospheric transmission on the summit of Mauna Kea in the specified frequency range for different Precipitable Water Vapor (PWV) values (computed using data from [6]).

(a) Microwave absorption due to atmospheric gases

(b) Microwave attenuation at various rain rate

Fig. 3.11.: Absorption and attenuation in the microwave range. Taken from [7].

2. For the millimeter range (1cm down to 1mm, or 30GHz to 300GHz) the picture is different: there are black areas for transmission due to the attenuation introduced by molecular absorption at several frequencies (see Figure 3.11(a)).
3. It is important to consider attenuation for the environment of study. Besides molecular absorption, there will be water droplets and aerosols (fog) as part of the firefighting procedures. An estimation can be done using the data shown in 3.11(b) for different rain rates.

The expected range of operation for applications in the scope of this thesis is in the meter range and therefore neither absorption nor attenuation will be the killer conditions of the system.

3.2.3. Data acquisition and limitations

The generation and detection of the returning echo will be one of the most challenging processes in the system. Here, the availability of pulsed optical sources is another advantage of optical frequencies.

Focusing on a laser-based system, it is necessary to name the Light Detection And Ranging (LIDAR), a remote sensing technology that measures distance by

illuminating a target with a laser and analyzing the reflected light⁵. The lidar⁶ equation accounts for the power received by a lidar system [129]. This equation is conceptually similar to the *Figure of Merit (FOM)* applicable to acoustic systems.

For the scattering mechanisms considered (Rayleigh and Mie), the lidar equation is fairly simple. In the case of a pulsed, monostatic lidar, the increment in signal power at the photodetector $\Delta P(\lambda, R)$ in the interval $(\lambda, \lambda + \Delta\lambda)$ from the element located at a range interval $(R, R + \Delta R)$ is given by

$$\Delta P(\lambda, R) = \int J(\lambda, R, \mathbf{r}) \Delta\lambda \Delta R p(\lambda, R, \mathbf{r}) dA(R, \mathbf{r}) \quad (3.34)$$

where:

- $J(\lambda, R, \mathbf{r})$ represents the laser-induced spectral radiance at wavelength λ , at position $\mathbf{r}$ in the target plane located at range R , per unit interval:

$$J(\lambda, R, \mathbf{r}) = \beta(\lambda_L, \lambda, R, \mathbf{r}) I(R, \mathbf{r}) \quad (3.35)$$

where

- $I(R, \mathbf{r})$ is the laser irradiance at position $\mathbf{r}$ and range R , and
- $\beta(\lambda_L, \lambda, R, \mathbf{r})$ is the *volume backscattering coefficient*, previously discussed.
- $dA(R, \mathbf{r})$ represents the element of target area dA at position $\mathbf{r}$ and range R ,
- $p(\lambda, R, \mathbf{r})$ represents the probability that radiation backscattered from target will reach the photodetector.

$$p(\lambda, R, \mathbf{r}) = \frac{A_0}{R^2} T(\lambda, R) \xi(\lambda) \xi(\mathbf{r}, R) \quad (3.36)$$

It depends on

- A_0/R^2 is the solid angle of acceptance of the receiver optics;
- $T(\lambda, R)$ is the atmospheric transmission factor;
- $\xi(\lambda)$ represents the receiver's spectral transmission factor and includes the influence of any spectrally selective component or filter;
- $\xi(\mathbf{r}, R)$, is the *overlap factor* and represents the probability of radiation from position $\mathbf{r}$ in the target plane at range R reaching the detector (geometrical considerations). For long-range operation it may be considered as 1, while not in the short-range mode of operation (which is our case).

⁵The development of *Q-switching* by McClung and Hellwarth [128] made it possible to generate very short pulses of laser, enabling range-resolved measurements in a similar manner to radar. The time passed from the transmission to the arrival can be related to the point where the scattering occurred.

⁶The acronym LIDAR is now used as a regular word and hence written in lowercase.

At time $t = 2R/c$ (round time for a pulse travelling at speed c that reaches a target at R), the total signal received is:

$$P(\lambda, t) = \int_0^{R=ct/2} dR \int_{\Delta\lambda_0} d\lambda \int J(\lambda, R, \mathbf{r}) p(\lambda, R, \mathbf{r}) dA(R, \mathbf{r}) \quad (3.37)$$

which accounts for all contributions of scatterers that reach the detector at time t .

The equation can be simplified if the medium is homogeneous, the pulse is square-shaped and a leading-edge detector is used. However, such assumptions cannot be made in general for the framework of this thesis.

There are other factors that are relevant in stating the final performance of a system, some of which are not considered by the equation and have to be taken into account for a final performance assessment. To name a few:

- **Signal processing techniques.** They may provide additional suppression of undesired responses and echoes, speckle, etc. Besides, they define how and when a certain received signal is considered to be the response from the target (decision process, probability of detection vs. false positives, etc.).
- **Optics.** Proper design of the lenses of the camera is crucial to get the maximum performance from a lidar system [130].
- **Controlling unit:** exact timing of the stages involved in obtaining an image is needed to avoid distortions and unwanted artifacts (clock jitter, lack of synchronization, etc.).
- **Photodetector.** The detection limit is linked to the photodetector used and its intrinsic features, which determine the ultimate performance achievable.

An important element to be analyzed is **noise**. Sources of noise can be endogenous (such as the ones related to the photodetectors themselves, like thermal noise) but they may also come from the outside (unwanted photons, etc.).

The most important sources of noise are:

1. *Photon counting noise:* The number of photons counted during a time interval is a random variable whose mean is proportional to the expected number of photons. The random element in the measurements reflects the fact that the photons arrive at random times, thus introducing uncertainty in the number of photons measured and therefore noise.
2. *Laser speckle noise:* Laser speckle noise effects are caused by interference from independent, individual scatterers occurring at the detector. The interference phenomenon occurs as the electromagnetic field from the illuminating laser reflects off an extended target surface.
3. *Thermal noise:* Anything that is not at 0K radiates photons. So any practical detector will generate noise. This parameter is assessed measuring the dark current of the system⁷.

⁷The “dark current” is the current measured at the output when there is no input.

Fig. 3.12.: Photodiode constituent materials as a function of wavelength. Taken from [8].

4. *Background noise*: In this context, it is constituted by any other light or signal that is collected by the detector and does not originate from the laser transmitter. For most practical scenarios, the background radiation is simply sunlight that falls on the detector. The background photons collected by the sensor bear no information concerning the range to the target, but the random arrival times of the photons from the background do contribute noise to the lidar system.

The electrical and physical characteristics of the sensing device are very important to be able to determine the noise profile and the ultimate capabilities of the lidar system. The sensing device converts the optical energy received (backscattered photons) into electrical energy [131] using *photodiodes*.

Photodiodes are semiconductor light sensors that generate current or voltage when illuminated by light. In general, they exhibit excellent linearity with respect to incident light, low noise and wide spectral response. They must be long-lasting and small while being mechanically rugged. There are several types of photodiodes attending to their construction and materials [8] (see Figure 3.12).

The low-light-levels inherent to remote sensing application make Avalanche Photodiodes (APDs) very interesting, as they are essentially detectors with gain (obtained usually by applying a high reverse bias voltage). In principle, any semiconductor material can be used.

3.2.4. Eye safety considerations

Operation safety is an important issue concerning use and implementation of systems that may expose the naked eye to radiations from a laser device. The coherence and low divergence angle of laser light, while being a desired feature

Tab. 3.4.: Pathological effects of overexposure to laser radiation.

Wavelength range	Pathological effect
180-315nm (UV-B, UV-C)	photokeratitis (inflammation of the cornea, equivalent to sunburn)
315-400nm (UV-A)	photochemical cataract (clouding of the eye lens)
400-780nm (visible)	photochemical damage to the retina, retinal burn
780-1400nm (near-IR)	cataract, retinal burn
1.4-3.0μm (IR)	aqueous flare (protein in the aqueous humor), cataract, corneal burn
3.0μm-1mm	corneal burn

in remote sensing, may pose high risks to unprotected users. Moderate and high-power lasers are potentially hazardous because they can burn the skin or the retina even faster than the blink of an eye (see Table 3.4) and hence cannot be used in search-and-rescue operations. Various specifications, for example ANSI Z136 in the US [132] and IEC 60825 [133] internationally, define several “classes” of laser depending on their power and wavelength.

The **Maximum Permissible Exposure (MPE)** is the highest power or energy density (in W/cm^2 or J/cm^2) of a light source that is considered safe, i.e. that has a negligible probability for creating damage. For artificial vision systems, IEC60825-1 classes (see Figure 3.13) up to Class 3R would be admitted. Note that other conditions may apply to pulsed lasers, so careful safety assessment of the chosen device, application scenario and pulse modulation should be conducted in order to ensure eye-safe operation.

3.2.5. Technology

A general scheme of a lidar system is depicted in Figure 3.14. In its simplest form, a laser pulse is sent and the time at which the received echoes from the scatterer arrive is measured with a counter. This way, a measurement of the Time-Of-Flight (TOF) is available and the range is determined. It is possible to obtain 3D images using this method, when many individual elements are grouped and combined (pixels).

There are several basic **types of imaging lidars** depending on how they obtain the information:

1. **Single-pixel scanning lidars.** They are based on successive measurements of range for individual points [134]. This type of lidar requires a moving mechanism to shift (scan) the aim point of the sensor over the area of in-

Fig. 3.13.: Maximal allowed CW-powers for the laser classes 1, 2, 3R and 3B according to the norm EN 60825-1:2007 (worst-case scenario).

Fig. 3.14.: Overview of a lidar system.

terest. They commonly consist of mirrors controlled electronically. There have been efforts in implementing such mirrors with *MicroElectroMechanical Systems (MEMS)* [135]. Other interesting alternatives include the use of polarization properties of *liquid crystals* [136]. Compressed sensing techniques [137] provide with another alternative solution to the use of moving parts.

Single-pixel systems are quite simple from the detector point of view, but they need an extremely careful design of the geometry of the system. Besides, it is quite limited if targets can be in motion because it takes $n_p f_r$ (where n_p is the total number of pixels and f_r is the frequency repetition rate) seconds to obtain an image.

2. **Gated viewing imagers** are another type of lidars [138, 79]. They open the detector during a certain time interval, that is, the receiver circuitry is “gated”, delaying its activation a certain time τ_a . This way it is possible to filter out undesired responses from fog, haze, etc. However, the range has to be set up by the user.

Replacing the single-detector element found in a simple rangefinder system with an array of detectors at the focal plane of the receiver, and controlling all of the elements with the same timing, it is possible to produce a 2D image of the target under observation. Besides, if multiple 2D slices are collected at a different range, a 3D image can be formed.

3. **Flash lidar.** This type of lidar has been introduced by Advanced Scientific Concepts [139] and combines the properties of conventional lidars with those of regular cameras [140]. Its principle of operation is quite simple, a single laser pulse illuminates (“flashes”) the scene with a laser pulse as if it were a conventional camera. Then, a 2D focal plane array of photodetectors measure the time it took the laser pulse to reach the target and return to the camera for every pixel and thus, for every element in the scene. This way the complexity of the detector is justified by the high frame rate of the camera, which can take pictures of moving objects.

In practice, the outgoing laser beam is formed so that the beam footprint on the target area closely matches the Field Of View (FOV) of the receiver. Depending on the range and number of pixels in the receiver, the outgoing beam may be reformed into beamlets [141] or into a uniform profile.

A modified flash lidar solution for artificial vision applications would be promising if the travelling signal and its postprocessing was able to overcome propagation distortions in the medium (scattering, etc.).

Fig. 3.15.: Simulated zenith atmospheric transmission on the summit of Mauna Kea in the THz band for different precipitable water vapor (PWV) values. Taken from [7].

3.3. Other options

Once the conventional approaches for mechanical and electromagnetic signals at optical frequencies have been presented, other technologies and research lines that may be relevant to artificial vision systems for temporary blind users will be discussed.

3.3.1. Terahertz

Terahertz is the frequency range that lies at the far end of the infrared band, just before the start of the millimeter microwave band. The term “terahertz” is used to refer to electromagnetic waves at frequencies from 0.3 to 3 terahertz (THz).

Technology for generating and manipulating terahertz radiation is a subject of active research. It represents the region in the electromagnetic spectrum where the frequency of electromagnetic radiation becomes too high to be measured using electronic counters, and must be measured by the properties of wavelength and energy. Similarly, in this frequency range the generation and modulation of coherent electromagnetic signals ceases to be possible by conventional electronic means, and requires new devices and techniques.

Terahertz radiation travels in a line of sight –as light– and can go through dielectric media up to a certain extent. It has the problem, however, of limited or poor propagation through water, fog or clouds, as shown in Figure 3.15 (using the same model as in Figure 3.10): transmission drops to 0% for PWV=5mm above 500GHz.

At distances of about 10 meters the band may still allow many useful applications in imaging and wireless networking due to their high bandwidth available. Sources of terahertz are scarce, but include FIR and quantum-cascade lasers which often need cryogenic cooling to compensate for the low energy of the photons at terahertz frequencies. These problems may pose a significant drawback when it comes to artificial vision through particle-filled atmospheres or mobile applications but there is margin for improvements [142].

There are also early efforts towards implementing practical solid-state terahertz imaging devices [143]. These prototypes work in the vicinity of 600GHz and can extend their working range up to 1THz with industrial CMOS technology, which opens the door to lower cost applications.

3.3.2. Metamaterials, subwavelength imaging and time-reversal mirrors

In the recent years, significant research has been done on investigating the properties and prospective uses of evanescent fields and waves. That effort has led to the development of 2D and 3D **metamaterials** [144] that are able to overcome diffraction limits of classical waves such as light or sound.

Diffraction sets a natural limit on how finely the details of an object can be recorded on its image. On the contrary, metamaterials are artificial materials engineered to have properties that are not found in Nature. They may be made of multiple individual elements arranged in periodic patterns that allow them gain properties not only from their composition, but from their exactly-designed structures. Their precise shape, geometry, size, orientation and arrangement can affect the waves of light or sound in an unconventional manner, creating materials with properties unachievable with conventional ones.

The evanescent components of a subwavelength feature or object can be transmitted efficiently through those specially crafted structures making acoustic imag-

ing possible at a very deep-subwavelength scale (on the order of $\lambda/50$) [145]. These properties can lead to huge improvements in the resolution of systems of a certain size or otherwise miniaturization of existing systems, a highly desired feature in our case.

Another interesting tool used to focus waves is the use of **Time-Reversal Mirrors (TRMs)**. The time reversal technique is based upon a feature of the wave equation known as *reciprocity*: If there is a solution to the wave equation, then the time reversed solution is also a solution. This occurs because the standard wave equation only contains even order derivatives. Some media are not reciprocal (e.g. very lossy or noisy media), but many can be approximated as so, including acoustic waves in water or air, ultrasonic waves in human bodies, and electromagnetic waves in free space. The medium must also be approximately linear. TRM can refocus an incident acoustic field to the position of the original source regardless of the complexity of the propagation medium.

Fink et al. [146] have been studying the properties of TRM for pressure (acoustic) waves, finding that the focusing is more precise when more scatterers are present in the cavity [147]. In addition, time-reversal mirrors can be iteratively applied for pulse-echo detection, overcoming the diffraction limits [148].

Despite being an active field of research, significant results have been obtained using **compressed image sensing** techniques [149] (see chapter 8).

3.4. Concluding remarks

The paragraphs above have shown the most relevant properties of electromagnetic and acoustic signals for the development of devices for use in particle-filled atmospheres. Acoustics works very well in underwater environments, with good resolutions if higher ultrasounds are employed (at the cost of higher attenuation). Remarkably, they have good performance when it comes to scattering for common environments –with clay or other dust-sized suspended particles–. Higher frequencies make it possible to reduce the size of the devices and improve their portability.

Electromagnetic signals at optical and infrared frequencies have the advantage of narrow beams and very high range resolution. Scattering is critical in their case, and devices should be designed taking into account the sizes of the suspended particles (in many cases comparable to the wavelength of the signals considered).

The development of systems able to overcome the challenges imposed by these scenarios need an in-depth knowledge of the basic properties of the signals used, together with a knowledge of the aberrations introduced by the medium. It is therefore convenient to study those media in depth in an effort to find their key features. Next chapter is devoted to this characterization.

4. The medium: characterization

“Everything must be made as simple as possible. But not simpler.”

Albert Einstein

One of the most difficult problems in pursuing artificial vision technologies in particle-filled atmospheres is undoubtedly the characterization of the medium in terms of propagation of the signals involved. It is therefore important to analyze the composition of the mediums proposed as cases of study (smoke and suspensions in water) in order to define a set of “typical conditions” and a set of representative parameters for them.

Our ultimate purpose would be to know which frequencies can traverse a particle-filled space in better conditions so that we can remotely sense the limits of that space and the objects therein. A study of different scattering theories and models applicable to the environments under study is necessary to better understand and characterize them.

4.1. Characterization of smoke

It is extremely difficult to define a standard medium when it comes to fire environments. The numerous substances present in different states of aggregation (solid, liquid, gas and plasma¹) combined with the many factors involved make characterization a very difficult task and, as a consequence, models are not widely applicable [151]. That being said, the aim of this section is to analyze smoke-filled atmospheres in order to extract a number of quantitative parameters (one may call them “typical fire conditions”) that could lead to shape a qualitative model of wave propagation.

In that sense, clean air will be studied first (Section 4.1.1), defining its molecular components and their relative concentrations along with their geometrical properties. Next, combustion products will be studied in Section 4.1.2. Last, particle

¹Although the temperatures commonly encountered in flames are not high enough to ionize the incandescent gases and thus generate a plasma, some fires may reach temperatures high enough to generate them. See [150], page 25.

Tab. 4.1.: Gaseous composition of dry air (% from [15]. Cross-sections computed from data in [16, 17, 18, 19]).

Molecule	Chemical symbol	Mole/Volume %	Cross-section "a" (pm)
Nitrogen	N ₂	78.084	250.00
Oxygen	O ₂	20.947	246.00
Argon	Ar	0.934	212.00
Carbon dioxide	CO ₂	0.0350	380.00
Neon	Ne	0.001818	116.00
Helium	He	0.000524	56.00
Methane	CH ₄	0.00017	278.05
Krypton	Kr	0.000114	232.00
Hydrogen	H ₂	0.000053	126.00
Nitrous oxide	N ₂ O	0.000031	374.00
Xenon	Xe	0.0000087	280.00
Ozone ¹	O ₃	trace to 0.0008	404.32
Carbon monoxide	CO	trace to 0.000025	248.00
Sulfur dioxide	SO ₂	trace to 0.00001	441.32
Nitrogen dioxide	NO ₂	trace to 0.000002	419.17
Water	H ₂ O	variable, typ. 1	245.58
Ammonia	NH ₃	trace to 0.0000003	262.63

¹: Low concentrations in troposphere.

size distributions of soot for different fire types will be obtained and discussed in Section 4.1.3.

4.1.1. Study of clean air

Air can be defined as a mixture of gases. Dry air [15] contains roughly (by volume) 78.09% nitrogen, 20.95% oxygen, 0.93% argon, 0.039% carbon dioxide, and small amounts of other gases. Table 4.1 shows the gaseous composition of air, along with the cross-section of the constituent molecules (see section 4.1.1.1). Air also contains a variable amount of water vapor, on average around 1%. Its composition varies locally though depending on other factors such as pollution, altitude or proximity to the sea –to name a few–.

There are software packages available (such as MODTRAN® [55]) that simulate electromagnetic wave propagation through the atmosphere, but they are not of direct application for the scope of this thesis (it is not intended for short distances, presence of smoke,...).

The interaction between incident radiation and particles has been extensively studied in particle physics, giving rise to several fundamental theories like Mie and Rayleigh theories already presented in section 3.2.2. Here we recall one of the most important parameters to predict the result of the interaction of the incident

wave with a certain particle, which is the size parameter α :

$$\alpha = \frac{2\pi a}{\lambda} \quad (4.1)$$

where λ is the wavelength of the incident wave and a the size of the particle. Hence, it is necessary to estimate the size of the molecules present in the air. It is also important to take into account that careful measurements for particular molecules give different diameters according to the experiment chosen and the method of interpretation used: recalling quantum physics, molecules are better described by statistics than by ball-like models. However, for the purposes of this thesis atoms will be approximated as spheres and molecules will be considered to have pure covalent bondings. Atomic data has been acquired from [16], and covalent bonding lengths from [17] (single), [18] (double) and [19] (triple).

4.1.1.1. Molecular cross-section

A new parameter called “*molecular cross-section*” has been defined conveniently as the molecule’s highest dimension. That dimension has been calculated as the length of the molecule in the case of linear molecules (nitrogen, oxygen, carbon dioxide, hydrogen, carbon monoxide, nitrous oxide and carbon monoxide) and as the highest 2D dimension of all the possible graphical projections of the molecule in the rest of the cases. Molecules will then be approximated by an *equivalent sphere* of diameter a , which will be used for scattering simulations.

Figure 4.1 shows the computation method for linear (oxygen, carbon dioxide, hydrogen, nitrous oxide and carbon monoxide), plane (sulfur dioxide, nitrogen dioxide, water) or tetrahedral molecules (methane, ozone, ammonia). Note that the resulting diameter will be equal to the cross-section for linear or plane molecules; for tetrahedral molecules $a = \frac{\sqrt{6}}{2}r$. Table 4.1 includes the computed values for the molecular cross-sections of the different molecules in air.

A plot of the resulting molecular size distribution is available in Figure 4.2, where it is clear that it is possible to model air as a gas consisting of molecules of sizes in the range 245-260pm.

4.1.2. Combustion products

In case of fire, there are many molecules that may be present as combustion products besides CO_2 and H_2O –which result from complete burning of hydrocarbons–. The presence and relative amount of those molecules depend on the material being burnt and the particular conditions of the combustion, specially ventilation. These conditions alter the chemical reactions in enclosure fires and lead to larger generation of soot (mainly made of carbonaceous particles) and other compounds (see [152]):

Fig. 4.2.: Molecular cross-section size distribution of clean air with water content about 1%. Data from Table 4.1.

- **Carbon dioxide** is the product resulting from complete burning in well-ventilated spaces. Nearly all the carbon lost from the combustibles is converted to carbon dioxide (CO_2).
- **Carbon monoxide** (CO) is produced from both smoldering and flaming combustion but in quantities much lower than carbon dioxide (ratios of 1:20 are common in well-ventilated environments).
- **Hydrogen cyanide** (HCN): its generation is both material and temperature dependent. In smoldering fires and pyrolysis from flaming fires, HCN can be produced by decomposition of some nitrogen-containing polymers. It has also been seen to be oxidized to NO_x when flames extended from a flashed-over room and continued to burn outside the doorway.
- **Halogen acids** (HF , Cl , Br , I): Polymer systems containing halogen atoms (fluorine, chlorine, or bromine) result in the formation of the halogen acids. The halogen acids are formed in the pyrolysis component of the combustion process and are not oxidized any further. Since the production efficiencies for the formation of HF , HCl , and HBr are close to being unity, maximum yields might be expected in fires.
- **Other inorganic irritants**, such as ammonia (NH_3) or sulfur dioxide (SO_2).
- **Organic compounds**: Pyrolysis and/or incomplete combustion of organic materials can lead to a wide variety of organic irritant species, among them

Tab. 4.2.: Approximate cross sections for different fire gases (using data from [16, 17, 18, 19] and Jmol).

Molecule	Chemical symbol	Cross-section "a" (pm)
Water	H ₂ O	245.58
Carbon dioxide	CO ₂	380.00
Carbon monoxide	CO	248.00
Hydrogen cyanide	HCN	323.00
Nitrous oxide	N ₂ O	374.00
Nitrogen dioxide	NO ₂	419.17
Hydrogen fluoride	HF	184.00
Hydrogen chloride	HCl	264.00
Hydrogen bromide	HBr	297.00
Hydrogen iodide	HI	335.00
Sulfur dioxide	SO ₂	441.32
Ammonia	NH ₃	262.63
Phosgene	COCl ₂	457.09
Acrolein	CH ₂ =CHCH ₃	490.70
Formaldehyde	CH ₂ O	329.09

phosgene, isocyanates and aldehydes (formaldehyde, acrolein). Other organic compounds, remarkably *Polycyclic Aromatic Hydrocarbons* (PAHs) are known to be pollutants and some of their compounds have been identified as carcinogenic, mutagenic and teratogenic (see section 4.1.2.1 below).

- **Other gases and aerosols**, depending on the substances being burnt.

Table 4.2 shows the calculated cross-sections for common combustion products computed using the same method as in Table 4.1. For more complex molecules such as acrolein, the Jmol [153] suite v.13.0 has been used, identifying the highest dimension in the 3D model.

4.1.2.1. Polycyclic Aromatic Hydrocarbons (PAHs)

Poly-aromatic hydrocarbons or polynuclear aromatic hydrocarbons have been subject of study as they can be carcinogenic or otherwise toxic. They consist of fused aromatic rings and do not contain heteroatoms or carry substituents. Toxicity of PAHs is deeply dependent on molecule spatial structure, with isomers (PAHs with the same formula and number of rings but different spatial setup) varying from being nontoxic to being extremely toxic. Thus, highly carcinogenic PAHs may be small or large. It is known that PAHs are released during incomplete burning of hydrocarbon fuels. Several studies have been conducted quantifying the presence and amount of PAH in smoke crude oil samples and oil burn residues [154, 155].

However, measurements of the geometry of PAH molecules are scarce, since

Tab. 4.3.: Approximate cross sections for different PAHs [using data from [16] and Jmol].

Molecule	Chemical symbol	Cross-section "a" (pm)
acenaphthylene	C ₁₂ H ₈	786
acenaphthene	C ₁₂ H ₁₀	789
fluorene	C ₁₃ H ₁₀	975
2-methylfluorene	C ₁₄ H ₁₃	981
phenanthrene	C ₁₄ H ₁₀	977
methylphenanthrenes	C ₁₅ H ₁₃	1026
dimethylphenanthrenes	C ₁₆ H ₁₆	977
anthracene	C ₁₄ H ₁₀	1009
fluoranthene	C ₁₆ H ₁₀	964
pyrene	C ₁₆ H ₁₀	1001
1-methylpyrene	C ₁₇ H ₁₃	1099
benzo[ghi]fluoranthene	C ₁₈ H ₁₀	960
cyclopenta[cd]pyrene	C ₁₈ H ₁₀	986
chrysene/triphenylene	C ₁₈ H ₁₂	1235
benzo[b]fluoranthene	C ₂₀ H ₁₂	1137
benzo[e]pyrene	C ₂₀ H ₁₂	1013
benzo[a]pyrene	C ₂₀ H ₁₂	1231
2-methylcholanthrene	C ₂₁ H ₁₆	1510
benzo[ghi]perylene	C ₂₂ H ₁₂	1039
indeno[1,2,3-c,d]pyrene	C ₂₂ H ₁₂	1162

they imply ultrahigh resolution like in [156] and the molecules are resonant in nature (the electron cloud in the molecule makes it even more difficult to obtain accurate values). An estimate of the size for different molecules is shown in Table 4.3.

4.1.3. Study of smoke particles: soot

The term "smoke" has been defined in the literature in different manners. The American Society for Testing and Materials (ASTM) defines it as the aerosol or condensed phase component of the products of combustion, including the evolved gases as well. This is in line with the preferred definition(s)² of smoke given by the NFPA [158]. Here, we will define smoke as the aerosol or *condensed phase* component of the products of combustion [9].

4.1.3.1. Soot formation

Many questions persist regarding the details of soot formation in its various stages. Despite significant effort has been made over the last decades (see the excellent

²The 2003 NFPA Glossary of Terms [157] showed a secondary but accepted definition of smoke comprising only the particulate, suspended in gases, vapors or solid and liquid aerosols.

review by Haynes and Wagner on the topic [159]) it is a relatively vivid research topic still today, spoiled in part by the ever increasing pressure that environmental regulations by the Environmental Protection Agency (EPA) in the US and the European Environment Agency (EEA) in the EU put onto Diesel engines designers [160].

Ian M. Kennedy has reviewed different models of soot formation and oxidation [161], focusing on the fundamental aspects of soot formation. From a purely chemical point of view, as hydrocarbons pyrolyze, they break and produce smaller hydrocarbons; in particular, ethylene and acetylene. The initial step in the production of soot is the formation of simpler aromatic species from these shorter hydrocarbons. The aromatic compounds grow by the addition of other aromatic and smaller alkyl species forming larger PAHs. Continued growth of PAHs leads to the smallest identifiable soot particles (*inception*), whose diameters are on the order of 1nm and their masses are around 1000amu³.

The process of particle inception and its later soot production is very complex and cannot be explained using thermodynamics alone. It is a kinetically limited process and hence both theories have to be accounted for to describe the reactions taking place in a plausible way [162]. The particles formed through the inception process grow by two main mechanisms: collisional coagulation and surface growth, being the first one physical and the second one chemical in nature. At the beginning, when particles are small, surface growth is dominant, with acetylene and PAHs playing an important role. Later, collisional coagulation becomes dominant. Many models have been developed. Ian M. Kennedy has grouped them into three main types: empirical correlations, semi-empirical models and models with detailed chemistry. The interested reader can find many references on the topic in [161].

This *agglomeration process* leads to the formation of chains of spherules whose individual diameters are in the range of 30-50nm. The agglomerates, however, exhibit variable geometries which have been modelled by several authors as fractal-like (see Figure 4.3). The morphology of those agglomerates plays an important role in the determination of relevant properties such as light scattering.

In the following sections, particle size distributions for different types of smokes, as well as optical properties of soot will be discussed. A reference will be made to the technology that has made possible advances in the matter.

³amu. – **atomic mass unit**, non-SI unit of mass (equal to the atomic mass constant), defined as one twelfth of the mass of a carbon-12 atom in its ground state. Used to express masses of atomic particles: 1amu $\approx$ 1.660538921(73)10⁻²⁷kg.

(a) TEM image taken from [163].

(b) TEM image taken from [164].

Fig. 4.3.: Typical Transmission Electronic Microscope (TEM) images of soot spherules and agglomerates from different combustions.

4.1.3.2. Characterization of smoke particle size distributions

In the last decades, there has been a significant interest to characterize smoke and its properties (mainly optical such as scattering, etc.) at certain wavelengths [165, 166, 167]. This is easily explained by the fact that the main aim of that research is to discriminate different types of smoke in order to identify its source [168, 169] and be able to decide whether to trigger an alarm or not. Today, characterization is an active subject of research with environmental monitoring purposes [170].

A different approach is needed here: the aim is to find out the particle size distribution for different types of combustion [171] that may provide us with relevant information of how a smoke-filled atmosphere will look like from the point of view of suspended particles, helping build “typical” or “worst-case” scenarios. This would eventually lead to a knowledge of the desired properties and hence a choice of the signals best suited to propagate through the medium with less affection.

Within this frame, the articles mentioned about fire detection just above ([168], but also [172, 173]) provide with valuable data about the physical properties of different types of smoke covering a representative amount of cases. That data is analyzed below, but it is convenient to explain first the methodology involved in such measurements to be able to evaluate its applicability in this case.

First, it is necessary to define a way of translating the observed irregular shape of the smoke particulate into *Aerodynamic Effective Diameters (AEDs)*. The conversion is made saying that two particles will have the same AED if their settling

Tab. 4.4.: Stage cutpoint size diameters for the cascade impactors in the articles reviewed (in μm).

Impactor model	Stage 1	Stage 2	Stage 3	Stage 4	Stage 5	Stage 6	Stage 7	Stage 8	Stage 9	Stage 10
Marple S-290 [174, 175]	21.3	14.8	9.8	6.0	3.5	1.55	0.93	0.52	-	-
MOUDI [176]	10	5.6	3.2	1.8	1.0	0.56	0.32	0.18	0.1	0.056

time in a fluid of density $1000\text{kg}/\text{m}^3$ is the same. The exact value is given by comparison with the time it takes to settle a smooth spherical particle with unit density. Particle size distributions are measured with cascade impactors although optical particle counters are also used. In the case of cascade impactors, each stage is characterized by its cutpoint diameter, defined as the AED collected with 50% efficiency.

Table 4.4 shows the stage cutpoint size diameters for different cascade impactors used in the papers. Some of the most relevant data obtained by scientists for the purposes of this thesis is summed up here:

- **Offshore oil burn** [154, 172, 155]. A medium size experiment was conducted in Ontario. There, oil was burnt in free air and smoke samples were collected using an helium balloon specially crafted for the experiment. The smoke yields were in the range of 14.8 to 15.5% of the mass of fuel burnt for fires with effective diameters over 10m, but more variable in smaller fires (8 to 15% for fires 7m in diameter). The size of the smoke particles were measured with a 8-stage cascade impactor able to measure particulate in the range from 0 to $10\mu\text{m}$.

It is important to point out that one of the experiments showed that 83% of the particulate was below $9.8\mu\text{m}$. The results are presented in Figure 4.4.

- **Cotton wick and non-flaming wood smoke** [168]. Several important conclusions can be drawn from this article. Smoke particle size distribution is known to follow a lognormal distribution [9]. Almost half (48%) of the total mass of the cotton wick particulate was found to have an AED below $0.056\mu\text{m}$. The mass mean aerodynamic diameter was $0.3\mu\text{m}$ with a geometric standard deviation of 1.9. For wood, only 2.2% of the total smoke mass had an AED below $0.056\mu\text{m}$, and the mass mean aerodynamic diameter was $1.6\mu\text{m}$ with a geometric standard deviation of 2.

Figure 4.4 shows data acquired with the two cascade impactors in Table 4.4 for different fires (crude oil, cotton wick and wood). Those measured distributions are compared with lognormal distribution data (*Mass Median Aerodynamic Diameter (MMAD)* and *Geometric Standard Deviation (GSD)*) from the fires presented above [173]. In order to present lognormal distribution data in a more comparable way, a simple trick has been applied to the data: the continuous lognormal distribution has been converted to a step function

Fig. 4.4.: Particle size distribution for crude oil, cotton wick and wood smoke: measured values vs. lognormal distributions.

with the steps corresponding to the stages of the cascade impactors.

- **Acetylene and ethylene** [177]. Soot particles from flaming acetylene and ethylene fires can be described as chain-like structures, called agglomerates as they are made up of smaller sphere-like structures with measured physical diameters about 20 to 80nm (see section 4.1.3.1). Thus, agglomerates can be in the range of 0.04 to 20 μ m. It is important to note that the acetylene spheres are about 30% bigger than ethylene ones. However, the resulting soot particles are similar in size. In this study the authors do not reflect the particle size distribution.
- **Several flaming and non-flaming fires.** Several authors have compiled particle size distributions for different types of fires. For instance, data from beech wood, cotton lamp wick, polyurethane, toast or cooking oil fires in the form of lognormal parameters as discussed above (MMAD and GSD) has been published in [173] and depicted in Figure 4.5. Despite being obtained under different conditions, the results are consistent with those provided in [178] and [9] or [166, 167].

Figure 4.6 shows a comparison between smoke from cellulosic and plastic materials, both from nonflaming and flaming fires. It is clear that there is a higher presence of bigger particles in plastic smokes than there is in wood smokes. In both cases flaming fires have lighter (smaller particles) smokes than nonflaming ones (pyrolysis).

For completion, data from [10] has been compiled and depicted. Figure 4.7 shows it.

The sizes of the particles have been found to span over several orders of magnitude, ranging from 0.01 μ m to 3-4 μ m, and in some particular cases up to 10 μ m. In line with common-sense observations, light smoke corresponds with fires whose smoke particle size distribution has most of its content under 1 μ m (toast, cotton wick, cigarette), while heavy smokes correspond to smoke particle size distributions with important content over 1 μ m and lognormal distribution tales reaching in some cases the vicinity of 10 μ m.

4.1.3.3. Aerosol particle analyzers

Advances in our knowledge of aerosols have come together with corresponding advances in technology and machinery, which in turn have made it possible to gather data as well as validate or refine theories. It is the case of particle analyzers: starting in the 1970's [179], they were able to measure light extinction or scattering properties combining electrical fields and vacuum chambers to isolate and immobilize particles and monochromatic light to measure scattering. This idea of the possibility of characterizing individual aerosol particles became reality almost twenty years later with the advent of realtime analyzers [180], where

(a) Toast, oil and dust.

(b) Beech wood, cotton wick, polyurethane.

Fig. 4.5.: Particle size distribution for beech wood, cotton lamp wick, polyurethane, toast, cooking oil and ISO dust: measured lognormal distributions.

(a) Douglas fir (pyrolysis, flaming) vs. Polyvinylchloride (pyrolysis, flaming).

(b) Beech wood, cotton wick, polyurethane.

Fig. 4.6.: Particle size distribution for Douglas fir, polyurethane, polyvinylchloride and cellulosic insulation: measured lognormal distributions for flaming and non-flaming (pyrolysis and smoldering) fires. Data from [9].

(a) Rigid polyurethane foam (nonflaming) vs. Polyvinylchloride (nonflaming, flaming).

(b) Wood (flaming, nonflaming).

Fig. 4.7.: Particle size distribution for wood and plastics (polyurethane, polyvinylchloride): measured particle size distributions for flaming and nonflaming fires. Data from [10].

Fig. 4.8.: Scheme of an aerosol particle analyzer.

scattering data are collected from single particles at several angular locations (see Figure 4.8).

Again, the main aim of those analyzers is to identify and/or characterize the particles in an aerosol –usually for environmental studies–. This fact implies that the vendors only provide with scattering data for the illuminating source in their equipment, so information is available for very few wavelengths. There are databases available in the Internet with scattering data for different kinds of particulate and dusts [181, 182, 183].

4.1.4. Light scattering and soot

The study of light scattering during combustion has been an active research topic due to the inherent hostile nature of fire when it comes to probing and measurements [184]. Indirect remote sensing using optical means has been the most used technique to measure variables such as particle size, shape, structure and others [185]: scattering is affected by all those variables and so it has been used to measure them indirectly.

Soot in combustion is mainly carbon (97-99% of the mass is carbon), although it contains other products discussed in previous sections (liquid PAHs, etc.). Besides, soot is porous and contain cavities. As a result, optical constants of soot may be different to those of pure amorphous carbon [186, 187]. Soot particle sizes are in the lower micrometer range and therefore they are at the same temperature of their surrounding atmosphere. This means that they emit radiation in the InfraRed (IR) regions of the spectrum.

Many authors have focused their research on soot optical constants in the IR band. Blokh obtained a formula to approximate the *complex index of refraction of soot* for λ from 1 to 6 μm [188]:

$$m = 1.6 + 0.3\lambda - i\lambda^{0.6}, [\lambda \text{ in } \mu\text{m}] \quad (4.2)$$

Another study by Chang and Charalampopoulos [189] provided expressions valid

for λ from 0.4 to 30 μm :

$$\begin{aligned} n &= 1.811 + 0.1263\ln\lambda + 0.027\ln^2\lambda + 0.0417\ln^3\lambda, [\lambda \text{ in } \mu\text{m}] \\ k &= 0.5821 + 0.1213\ln\lambda + 0.2309\ln^2\lambda + 0.01\ln^3\lambda, [\lambda \text{ in } \mu\text{m}] \end{aligned} \quad (4.3)$$

The actual refractive index of soot is a function of a number of parameters. It will vary with carbon to hydrogen ratio in the soot, which will in turn depend upon the original fuel and oxidant combination and the age of the soot.

It is of prime importance to treat soot aggregates correctly: the scattered intensity increases due to irregularity caused by agglomeration, and Rayleigh scattering cannot be assumed unless certain degree of error is accepted [190]. There are cases, such as soot generated during the gas-phase combustion of volatile matter, in which it forms a concentric “mantle” around the parent coal particle. In this case, *modified Mie solutions* apply –for instance, using an effective complex index of refraction for the soot cloud obtained from Maxwell-Garnett theory–. It is important to remark that this approximation focuses on macroscopic properties of soot (soot cloud).

For individual particles, Mie theory is *strictly* valid only in the case of perfect spherical particles, which is not the case of soot aggregates. The **T-Matrix theory**, on the other hand, holds for a much wider range of particle shapes [191]. Both theories need the following as input parameters: complex index of refraction, particle size, wavelength of incident radiation and, for T-Matrix theory, the particle shape. For a polydisperse aerosol, responses from different particles can be linearly combined.

The particle size parameter α (see section 3.2.2) is a good approximation to determine the most adequate light scattering theory to use –see Figure 3.7–. In general, geometric scattering will be sufficient for $\alpha \gg 1$, Rayleigh scattering will hold well for $\alpha \ll 1$, and Mie or T-Matrix theories will outperform those when $\alpha \approx 1^4$. It is possible to predict angular light scattering intensity or phase function among many other properties [192, 193].

4.1.4.1. Mie and T-Matrix light scattering theories. The coupled dipole approximation

The purpose of this section is by no means to derive Mie or T-Matrix theories rigorously, but to present their relative strengths and weaknesses related to soot and smoke characterization. The interested reader is pointed to the work by Bohren and Huffman [194] (Mie theory) or [195, 196, 197] for T-Matrix.

Mie theory is the solution to the wave equation for plane electromagnetic waves scattering from a sphere. Its application to non-spherical particles and aerosols

⁴Note: Both Mie and T-Matrix theories converge to Rayleigh or geometric scattering for appropriate values of α .

means errors, although it still provides a first-order approximation in those cases. The relationship between the light incident on a particle I_i and the light scattered I_s can be expressed in terms of the scattering matrix S :

$$I_s = SI_i \quad (4.4)$$

This relationship can be expanded using the Stokes parameters (I , Q , U and V):

$$\begin{pmatrix} I_s \\ Q_s \\ U_s \\ V_s \end{pmatrix} = \begin{pmatrix} S_{11} & S_{12} & S_{13} & S_{14} \\ S_{21} & S_{22} & S_{23} & S_{24} \\ S_{31} & S_{32} & S_{33} & S_{34} \\ S_{41} & S_{42} & S_{43} & S_{44} \end{pmatrix} \begin{pmatrix} I_i \\ Q_i \\ U_i \\ V_i \end{pmatrix} \quad (4.5)$$

The scattering or Müller matrix S is determined by the characteristics of the medium, in this case the particle size, structure, symmetry, orientation and complex refractive index [198]. For randomly oriented aerosol particles, the eight off-diagonal block elements of the Müller matrix are zero. Of the remaining elements, S_{11} is proportional to the total scattered intensity, S_{22} is shape dependent, and the others have the following relationships: $S_{12} = S_{21}$, $S_{33} = S_{44}$ and $S_{34} = -S_{43}$. Values of S_{22}/S_{11} less than 0.9 at 120 degrees imply that the Mie analysis is not appropriate [199].

For a spherical scattering particle the coefficients can be determined analytically. In general, as the diameter of the scattering particle increases there will be an increase in the ratio of forward to backward scattering. Scattering phase functions of larger particles will also have narrower forward scattering peaks. It has been found that large non-spherical particles scatter similarly to area-equivalent spheres near the forward dimension whereas the differences between them become bigger for bigger angles. There is code available in the Internet to perform these calculations [200, 201].

T-Matrix theory is an exact *numerical* solution to Maxwell's equations for scattering from an object of arbitrary shape. Based on solutions to the integral formulation of Maxwell's equations, it was derived by Waterman between 1965 and 1971.

A particle of arbitrary shape is located at the origin of a spherical coordinate system with a plane wave incident upon it. The incident and scattered fields are then represented as a series of harmonics. Due to the linearity of Maxwell's equations it is possible to relate the incident field coefficients a , b to the scattered field coefficients p , q . In matrix form:

$$\begin{bmatrix} p \\ q \end{bmatrix} = T \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} T^{11} & T^{12} \\ T^{21} & T^{22} \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} \quad (4.6)$$

The T-Matrix depends only on the physical properties of the scattering particle, so once known it is possible to calculate the scattered light for any orientation of

incident radiation. Truncating the series that represent the internal field and relating the expansion coefficients of the internal field to those of the incident and scattered fields through a transformation matrix called Q , it is possible to reduce the infinite number of elements of Q and T to a finite, determinable problem. T can be greatly simplified if an ensemble of randomly oriented particles is assumed: in that case, T is diagonal. Otherwise, scattering for individual agglomerates is affected by the structure of the cluster and its particular orientation [202].

There is T-Matrix code publicly available in the Internet, remarkably in [203]. This code can be used to calculate the full scattering matrix as well as characteristic dust optical properties such as total extinction for randomly oriented particles of certain shape. The code takes as input parameters the wavelength of incident radiation, index of refraction of the particle, size distributions (as lognormal) and particle shapes based on ellipsoids. Besides, shape distributions -weighted- can be introduced. It is important to take into account that carbon aerosols are highly fractal in nature and therefore may not fit spheroids as close as other types of dust, although they are still a good approximation.

A significant limitation of this code is the finite maximum size parameter for which the code will converge. The computational load imposed by the code is much bigger than for Mie simulations, specially when highly eccentric particles are simulated.

Another light scattering model is based on the **coupled dipole approximation** [11], which assumes that each primary particle is a dipole oscillator. In this model, discrete elements are placed on a cubic lattice approximating the shape of the particle of interest. Each element is treated as a spherical, dipolar oscillator with a scalar polarizability. Interactions are accounted for by summation, which leads to large sets of equations that must be solved for the electric field of each oscillator. The accuracy of this method has been found to be dependent on the size of the dipole element with respect to the wavelength of the incident light: values deviate from Mie calculations when individual dipoles are larger than one tenth of the incident wavelength [204].

4.1.4.2. Fractal considerations for soot particles

There are a number of approaches towards modelling the scattering of particle aggregates. One of them is the couple dipole method presented in the previous section. It is less complicated but still requires a lot of computing power and an exact knowledge of the position of every spherule in the agglomerate (which is usually done simulating the aggregation process as well). Another option is to use full interactive scattering, which is seldom used due to its high computing requirements [205].

A simpler approach assumes that the incident wave may propagate undis-

turbed and then the *Rayleigh-Gans-Debye (RGD) approach* may be used [185]. Its basic assumption is that light is not reflected at the medium-particle boundary nor is it attenuated within the particle. Within this assumption each small portion of particle is subject to the same electromagnetic radiation conveyed by the incident light and scatters light as if isolated from the rest of the particle. There is a fractal version of this theory, the so-called *Rayleigh-Gans-Debye-Fractal-Aggregate (RGD-FA) approach*. The interested reader is pointed to the interesting review by Sorensen [206]. The different approaches to the fractal aggregate problem are being studied these days in order to assess its limitations and valid ranges [207, 208, 209].

In the RGD method the scattering is described in terms of the *scattering wave vector* $\mathbf{q}$, whose magnitude is:

$$q = \frac{4\pi}{\lambda} \sin \frac{\theta}{2} \quad (4.7)$$

where θ is the angle between incident and scattered directions. For N scatterers, the intensity becomes:

$$I(q) = \left| \sum_{n=1}^N e^{iqr_n} \right|^2 = \sum_{n=1}^N \sum_{m=1}^N e^{iq(r_n - r_m)} \quad (4.8)$$

where r_n is the position of the n -th particle.

If the positions of the individual particles of the agglomerate are not known, it is still possible to describe the agglomerates as fractal structures defined by

$$N = K \left(\frac{R_g}{a_p} \right)^{D_f} \quad (4.9)$$

where R_g is the radius of gyration⁵, a_p is the radius of the primary particles (spherules) and N is the number of primary particles in the agglomerate. K is a constant prefactor and D_f is the dimension: $D_f = 1$ for infinite cylinders, $D_f = 2$ for flat discs and $D_f = 3$ for spheres. For soot agglomerates the “fractal dimension” D_f is not an integer and has been found to be about 1.8 [210].

It has been seen that the RGD approximation works reasonably well for $D_f < 2$ [211, 212]. For $D_f > 2$ the agglomerate is too dense and the aggregate is better described by full interactive scattering (rigorous theory). Mie theory can be used when D_f is closer to 3. However, soot agglomerates are not pure fractals. If the fractal scale is small, the scattering due to individual particles may account for the most significant part. If the scale is very large, it can be outside the limits of

⁵**Radius of gyration or gyradius** is the name of several related measures of the size of an object, a surface, or an ensemble of points. It is calculated as the root mean square distance of the objects' parts from either its center of gravity or a given axis.

Tab. 4.5.: Overfire soot agglomerate parameters for different types of fuel.

Fuel	d_p (nm)	$\bar{N}$	D_f
Gas fuelled flames:			
Acetylene	47	417	1.79
Ethylene	32	467	1.80
Propylene	41	460	1.79
Butadiene	42	–	1.79
Liquid fuelled flames:			
Benzene	50	552	1.77
Toluene	37	–	1.80
n-Heptane	35	260	1.79

the actual aggregate. Hence, the correlation function has to be multiplied by a cut-off function [206].

Initially R_g is small and D_f relatively large (about 25nm and 2.55 respectively). In this region, the primary particles are either still separate or in their very first stages of agglomeration (hence $D_f \approx 3$, which is the value for spheres). As agglomeration progresses, R_g grows and D_f falls (380nm and 1.2, respectively). In this stage the agglomerates are similar to segments (or chains, hence $D_f \approx 1$). The agglomerate then begins to change shape, with R_g falling to about 160nm before further growing to about 280nm and D_f taking the value of about 1.9. The reasons why this restructuring occurs are still under study. Table 4.5 shows the values of d_p (diameter of the primary particle), D_f and $\bar{N}$ for different fuels as an example (after [213]).

Further studies have been made on other important variables such as scattering and extinction cross-sections [204]. It was found that scattering matrix parameters S_{12} and S_{34} are more sensitive to fractal properties than S_{11} [214, 215]. In addition, Mengüç noted in [216] that N and d_p may be obtained from the angular variation of S_{11} if the complex refractive index is known.

All these studies suppose that the primary particles are equal in size. But, *what happens if both particles and agglomerates have size ranges?* Polydispersity has implications if the standard deviation of the distribution is greater than 0.1. It is known that the effects of polydispersity can be neglected if the standard deviation of the distribution is less than 0.6, otherwise the assumption of monodispersity will underestimate the real part of the refractive index and overestimate the imaginary part. Besides, other effects such as the fact that particles may overlap may be important (the RGD-FA models assume that the particles are just touching each other). In this line, penetration factors have been proposed

$$C_p = (d_p - d_{ij})/d_p \quad (4.10)$$

–here, d_p is the primary particle size and d_{ij} is the distance between those two

Fig. 4.9.: Arrangement of dipoles on a lattice as dipoles are removed by random selection. The circular line represents the sphere used in the Mie calculation that best fits the scattering matrix elements. Taken from [11].

particles—, in order to adjust the fractal prefactor:

$$K = 1.3e^{2.2C_p} \quad (4.11)$$

Using the *coupled dipole method*, P. Hull et al. [11] were able to validate the Mie model for soot particles (porous clusters of particles with non-spherical symmetry and orientation averaging). She started with a 100% filled sphere and proceeded to remove spherules at random (see Figure 4.9). The deviation of S_{22}/S_{11} from 1.0 began to be noticeable, but still did not drop from 0.90. Another set of experiments was made using ellipsoids instead of spherules, yielding a surprising result: S_{22}/S_{11} increased as the ellipsoid become more porous (always being over 0.95). In conclusion, *it is possible to use Mie calculations as good approximations when S_{22}/S_{11} does not drop below 0.9*. This holds for randomly filled, spherule-filled spheres with a filling of only 20%. The match is better at angles lower than 90° .

4.1.5. Considerations on the motion of the molecules and smoke particles

It is important to take into consideration the fact that the atmosphere and, more specifically, smoke atmospheres are not static systems. The interactions between incident radiation and the particles in the atmosphere under study are more a subject of particle physics. This is the reason why it is important to study the motion of those molecules and other sorts of particles in order to find out if the effects of fire dynamics can be neglected (or not) for the application subject of this work.

The first thing to consider is the motion of the molecules of air and other combustion byproducts. It can be modelled using **kinetic theory** [217], which is a theory that describes a gas as a large number of atoms or molecules that move randomly and collide with each other and the walls of the container. The theory is only applicable to ideal gases, although real gases follow this theory provided

Tab. 4.6.: Speed of hydrogen molecules at different temperatures.

Temperature (K)	Speed RMS (m/s)
300	60.92
600	86.16
900	105.52
1200	121.85

that three necessary assumptions apply: the absence of quantum effects, molecular chaos and small gradients in bulk properties. Interestingly, macroscopic properties (volume, pressure, etc.) can be explained using kinetic theory. Deriving from kinetic energy, the Root Mean Square (RMS) speed of a particle can be expressed as:

$$v_{\text{rms}}^2 = \frac{3RT}{\text{molar mass}} \quad (4.12)$$

where T is the temperature and R is the universal gas constant.

The previous expression allows us to compute the speeds of the atoms and molecules present in the atmospheres in our scenario of study. The worst-case scenario is the most distant from the static case. Taking into account that $R = 8.3144621 \frac{\text{J}}{\text{Kmol}}$ and a molar mass of 2.016 kg/mol , substituting in the formula above, v_{rms}^2 will be higher at higher temperatures and for lighter molecules and atoms, so the molecule traveling at highest speed will be hydrogen (see Table 4.6).

In the case of electromagnetic waves, even at very high temperatures (1200K), the fastest molecule will travel almost 6 orders of magnitude slower than the speed of light (121m/s vs. $3\text{E}8\text{m/s}$). However, in the case of mechanical waves such as pressure waves, it is important to consider the possible effects of the movement of the molecules at temperatures over 300K (60.92m/s vs. $\approx 340\text{m/s}$). In practice, the size of the molecules in the medium compared to the incident wavelength (in both electromagnetic and acoustic cases) gives negligible scattering.

4.1.5.1. Brownian motion and smoke particles

While the particles that constitute a gas are too small and fast to be visible, the motion of other suspended particles such as soot or dust can be seen under a microscope or even by the naked eye. This random motion, known as Brownian motion, results directly from collisions between the particles and gas molecules (see an introduction in [218]). Given that the movement of molecules is random, so is the movement of the particle: the direction of the force of atomic bombardment is constantly changing, and at different times the particle is hit more on one side than another, leading to the seemingly random nature of the motion [219].

Besides, smoke aerosols are dynamic with respect to their particle size distribution function. Particles undergoing Brownian motion collide and stick together. The result of this behavior is that, in a smoke-filled volume, the number of particles decreases while the total mass of the aerosol remains unchanged. This process is known as **coagulation**.

Applying the same formula as in the previous section to compute the RMS speed of a smoke particle gives:

$$v_{\text{rms}} = \sqrt{\frac{3RT}{\text{molar mass}}} \quad (4.13)$$

which means that:

$$\frac{v_{\text{soot}}}{v_{\text{H}_2}} = \sqrt{\frac{m_{\text{H}_2}}{m_{\text{soot}}}} \quad (4.14)$$

Given the size and mass of soot agglomerates, it is easy to think of v_{soot} being several orders of magnitude lower than v_{H_2} , in the order of cm/s to m/s, depending on other factors. In fact, some of the collisions will tend to accelerate the particle undergoing Brownian motion; others will tend to decelerate it. If there is a mean excess of one kind of collision or the other to be of the order of 10^8 to 10^{10} collisions in one second, then the velocity of the Brownian particle may be anywhere between 10 to a 1000cm/s. Under those circumstances ($c \gg v_{\text{soot}}$, $c/v_{\text{soot}} \approx 10^8$), it is possible to neglect the movement of soot particles during the signal roundtrip and thus consider the proposed scenario as being quasi-static. This approximation will not introduce relevant errors and will simplify the model of the medium ("*quasi-static approach*").

However, movement should be considered if acoustic signals are used. In this case, the propagation speed in air is $v_a \approx 340\text{m/s}$ —depending on the properties of the medium—, so the approximation $v_a \gg v_{\text{soot}}$ is no longer valid unless a certain amount of error is assumed.

4.2. Characterization of turbid water

Once smoke-filled atmospheres have been studied, it is the turn for the second case of study proposed: the characterization of turbid water.

Underwater vision is confronted with similar problems to those presented for through-smoke vision. The presence of particles in suspension causes the incident radiation at visible frequencies to scatter preventing divers to see. However, the contour conditions are different and therefore some of the problems encountered in smoke will not be present here (high temperatures, presence of different types of fluids,...) and vice versa (liquid instead of gas).

4.2.1. Study of clean water

The study of pure water can be seen as a subset of the study of clean air from the point of view of particle size distribution, since pure liquid water is a fluid made only of water molecules, whose geometrical properties are shown in Table 4.1 (molecular cross-section of 246pm).

All non-ionizing electromagnetic signals under study will travel through water with little scattering and hence will not pose significant problems from that point of view. It is important to note, however, that they can suffer from other problems, such as refraction if the incident radiation goes through layers of different temperature. In general, for normal vision ranges –and excepting thermoclines– this should not be an issue (water can in general be considered homogeneous in ranges of tens of meters).

4.2.2. Study of particle suspensions in water: mineral dust

Particle size, also called grain size, refers to the diameter of individual grains of sediment, the lithified particles in clastic rocks, microscopic algae, krill, detritus or other biological material. Granular material can range from colloidal particles with sizes less than 1µm, through clay, silt, sand, and gravel, to boulders. We will consider only particles in suspension with sizes under 60µm.

There are two different acknowledged scales to classify granular materials:

- **ISO 14688-1.** From [220], ISO 14688-1, together with ISO 14688-2, establishes the basic principles for the identification and classification of soils on the basis of those material and mass characteristics most commonly used for soils for engineering purposes. ISO 14688-1 is applicable to natural soils in situ, similar man-made materials in situ and soils redeposited by man. See Table 4.7.
- **Krumbein ϕ Scale.** It is a modification of the Wentworth scale created in 1963 by W. C. Krumbein; it consists in a logarithmic scale computed by the equation

$$\phi = -\log_2 \frac{D}{D_0} \quad (4.15)$$

where D is the diameter of the particle in mm and D_0 is the reference, 1mm, so that the equation is dimensionless. The scale can be seen in Figure 4.10.

The sizes of mud particles for typical rescue diving have been found to reach 20µm (clay to fine silt), and in some particular cases up to 60µm (coarse silt).

The analysis conducted before for smoke particles is valid here as well, with the relative advantage that “problematic” particles will be in the size range pointed out above: there are usually no smaller particles, on the one hand, and on the other, bigger ones tend to fall and settle in a short period of time.

Fig. 4.10.: Krumbein/Wentworth ϕ scale. Taken from [12].

Tab. 4.7.: ISO 14688-1: basic principles for the identification and classification of soils.

Name		Size range
Very coarse soil	Large boulder, LBo	> 630mm
	Boulder, Bo	200 – 630mm
	Cobble, Co	63 – 200mm
Coarse soil	Gravel	Coarse gravel, CGr
		Medium gravel, MGr
		Fine gravel, FGr
	Sand	Coarse sand, CSa
		Medium sand, MSa
		Fine sand, FSa
Fine soil	Silt	Coarse silt, CSi
		Medium silt, MSi
		Fine silt, FSi
	Clay, Cl	

4.2.3. Light scattering and mineral dust

Numerous authors have focused their research towards the study of mineral dust aerosols. As a result, it is possible to conduct an analysis much similar to the one carried on for smoke.

Mineral dust has a high variability in terms of particle sizes and compositions. Despite this fact, particle size distributions have been modeled [221]. Remarkably, they do not follow lognormal distributions as in smoke. The radiative properties of mineral aerosols have been also modeled for various frequencies [222], in some cases incorporating the mineralogical composition [223].

It is not possible to define a set of typical properties due to the variability of refraction indexes and shapes of the particles depending on their constituents, although complex refractive indexes have been subject of study [224] –like in the case of smoke–. Optical properties of mineral dust have been also considered for specific dust compositions and sizes, such as clay [225]. Mineral dust aerosols have different compositions depending on the geographical area of the world (Asia, Africa, etc.). In addition to airborne dust, seawater dust [226] has been studied.

It is therefore possible to define the optical and geometrical properties of a particular type of dust. Once the dust has been parameterized, the model developed in the next chapter for smoke should hold for mineral dust, as well as for other types of particles. However, we have focused our research on smoke atmospheres, leaving mineral dust as future work.

4.2.4. Considerations on the motion of suspended particles

As in the case of smoke, suspended particles in water move following Brownian motion. The derivation is very complex [227], but it is possible to say that the speed of particles in water will be smaller than that for smoke particles in air.

This last fact makes it possible to neglect the movement of suspended particles in water for our purposes and consider this proposed scenario as static if the sensing process is made using electromagnetic signals ($c \gg v_{\text{particle}} \approx 10^8$). In this case, this approximation will not introduce relevant errors and will greatly simplify the computational model of the medium.

As for the case of smoke, movement should be considered if acoustic signals are used. In this case, the propagation speed in water is $v_a \approx 1440\text{m/s}$ –depending on the properties of the medium–, so the approximation $v_a \gg v_{\text{soot}} \approx 1\text{m/s}$ is valid assuming certain amount of error.

4.3. Concluding remarks

In the previous sections, an in-depth study of the optical properties of smoke has been conducted. A shorter but parallel analysis has been done for the underwater case of study. This way, we have been able to separate the analysis of the suspended particles (soot, dust, etc.) from their surrounding atmospheres (combustion atmosphere, water) providing with elements necessary to discriminate the appropriate scattering mechanism for each case and type of incoming signal involved. Despite the profound differences between the two cases, we have been able to give them an homogeneous treatment. This effort will open the door to a generalist framework model able to handle very different scenarios with a uniform approach and little to no adaptation.

5. A model for the simulation of particle-filled environments

“Science is what we understand well enough to explain to a computer. Art is everything else we do.”

Donald Knuth

Once certain knowledge has been gathered on particle-filled atmospheres, it is time to present a model that has been primarily developed for smoke filled atmospheres. The model has been conceived as a framework model, which means that it allows the user to simulate arbitrary smoke types and compositions by feeding the model with suitable data. This behavior can be easily extended to mineral dusts or other particle suspensions in water as well as long as the optical properties of the particles involved are known and therefore can be fed into the model. However, this and other extensions have been left as future work.

The approach followed in the development of this model is inspired in [228], although major adaptations and changes have been introduced to fit the intended applications. Before conducting real-world experiments, numerical simulations are proposed to gather some insight into concrete setups from both quantitative and qualitative points of view.

In the following chapters and sections we will focus on smoke; it must be understood that an analysis parallel to the one given to smoke would hold for mineral dust in underwater environments or other particle-filled atmospheres.

5.1. Related work

As presented in the previous chapters, studies of propagation of electromagnetic waves –such as light– in turbid media like smoke and soot-containing aerosols reveal the complexity of the problem. Analytic solutions are not available for the general case and other, more realistic models become rapidly intractable and hence models in this subject are scarce.

In the last years an important amount of the research in fire safety and engineering has focused on topics such as Computational Fluid Dynamics (CFD) [229], in

particular the development of new numerical methods or the improvement of existing ones. Other researchers have studied smoke plumes [230] or the effect of heat in compartment fires and its consequences on materials [231], etc.

The main purpose of the model presented here is to describe not only qualitatively, but also quantitatively, the propagation of electromagnetic signals at optical or infrared frequencies through a smoke-filled atmosphere over short distances (tens of meters, enough for artificial vision and the applications considered). Instead of focusing on the properties and possible consequences of the movement of smoke and hot gases in a fire scene, a novel perspective is explored: the smoke will be considered to be static due to the difference in the speeds of the agents involved ("*quasi-static* approach", see section 4.1.5). The propagation of electromagnetic signals in these conditions will be studied and modeled.

5.2. General model overview

The model described here takes a Monte Carlo approach which is simple in conception, but general enough to treat inhomogeneous smokes and effects such as absorption [232].

The model is built upon several parts (or models) related one another. Concept blocks and "submodels" are shown in Figure 5.1 and described below:

- An *optical model*, which characterizes the properties of the elements that affect the propagation of the incident wave. The medium (smoke) model is an optical model.
- A *geometrical model*, which describes the physical limits and shape of the elements involved: the physical limits of the simulation environment, called "space geometry", as well as the "emitter/receiver geometry" which sets the properties of the wave source and detector. The solid objects that the incident wave may find in its way are modeled as "object geometry" and comprise a mixture of optical and geometrical properties. For completion, both will be discussed when dealing with the geometrical model.
- A *propagation model*, the core of the Monte Carlo method, which describes how the incident wave interacts with the particles of smoke, and other physical entities in the simulation environment (simulation space boundaries, objects or sensor).
- A set of *physical fire conditions*, necessary to generate the concrete optical parameters for the model.

The model needs a number of parameters and contour conditions to be set by the user. A general overview of the actual input data needed by the model has been shown in Figure 5.2. The input data is classified as medium-related data (which includes data feeds for the optical model and physical fire conditions),

Fig. 5.1.: Smoke model: general overview.

Fig. 5.2.: Input data needed by the model.

environment-related data (including data feed for the geometrical model), and emitter/sensor-related data (which includes data for the geometrical model as well as for the optical model).

The approach used for the model is “event-based” in the sense that the light source is packetized in so-called **photon bundles** that travel through the scattering media. While close to ray-tracing in spirit, it differs from it in that the bundle is propagated in only one direction, which is chosen probabilistically in agreement with the scattering profile of the particles encountered (soot). This approach requires a significant amount of processing power but is partially overcome by the fact that every and each photon bundle is independent from any other of its neighbors, thus allowing for parallelization.

The photon bundles are simply a way to discretize the intensity emanating from every element in a pixelized 2D array serving as the source (which will be a monochromatic light source in our case, although more complex illuminating patterns can be considered making use of the superposition principle). This is

what will be called pixel intensity (see section 5.4.2). It can be expressed as:

$$i(x, y) = \frac{I(x, y)}{N} \quad (5.1)$$

where I is the total intensity from a given pixel and N the number of bundles per pixel. This discretization has the advantage of being able to derive rapidly coarse results by choosing smaller values for N and then go for finer results with $N' > N$. This procedure involves scaling the receiving pixels by N/N' and repeating the simulation with

$$i'(x, y) = \frac{I(x, y)}{(N' - N)} \quad (5.2)$$

5.3. Optical model

The optical model comprises the model of smoke as a set of particles, and the model for the behavior of the smoke particles themselves. Both are discussed below.

5.3.1. Smoke model

The main parameter of the smoke or particle-filled atmosphere (medium) when it comes to signal propagation will be the Mean Free Path (MFP) between particle and particle of soot and will be represented by

$$\bar{\Lambda} = \mathbb{E}\{\Lambda\} \quad (5.3)$$

Using the definition in [233, 234] as a first-order approximation –valid for the case of non light absorbing particles ($m = 3$)–:

$$\Lambda_{(MFP)} = \bar{\Lambda} = \frac{2d}{3\phi Q_{sca}} \quad (5.4)$$

where d is the diameter of the particle, ϕ is the volume fraction of the particles and Q_{sca} is the scattering efficiency¹.

The actual distance Λ between particles of soot will be modelled as an exponential variable with $\bar{\Lambda}$ mean. The realizations of the random variable will be computed using the inversion method by Devroye [236, 237]. For this case (exponential random variable with rate $\lambda = \frac{1}{\bar{\Lambda}}$) we have that

$$f^{-1}(U) = -\bar{\Lambda} \log(U^k) \quad (5.5)$$

¹Is is important to recall that the scattering efficiency relates the scattering cross-section to the physical cross-section. See [235] for details.

where U^k is the k -th realization of a uniformly distributed random variable.

It is even possible to treat inhomogeneities in the medium introducing a factor α , defined as

$$\alpha = \frac{\overline{\Lambda}^{k+1}}{\overline{\Lambda}^k} \quad (5.6)$$

or defining different MFPs depending on the region of the environment considered. Therefore, if the current (k -th) step is w^k , the “next” random step can be expressed as:

$$w^{k+1} = \alpha w^k \quad (5.7)$$

5.3.2. Modelling smoke particulate: scattering profiles

Once the incident radiation reaches a particle, it is scattered. The scattering will be treated in spherical coordinates (ρ, ϕ, θ) as follows:

- ϕ will be a uniform variable $[0, 360)$ such that:

$$\phi^{k+1} = 360U^k + \phi^k \quad (5.8)$$

- θ will be defined by the scattering profile of the particle reached by the incident wave and will have variability in $[-180, 180)$:

$$\theta^{k+1} = \sigma^k + \theta^k \quad (5.9)$$

where σ^k is a random variable distributed according to the scattering profile and generated by the inverse Cumulative Distribution Function (CDF) method.

5.3.2.1. Support for heterogeneous types of particles

It is interesting to have the possibility of including several types of particles with different optical properties in the same medium. At the cost of a slight increase in computational load, it makes the model much more flexible and adaptable to real environments.

The feature works as follows: it is possible to create a random variable whose CDF matches the relative size concentrations of the particles using a map function. A scheme of the technique used here is depicted in Figure 5.3 and provides with a fast and reliable form of generating random variables with a given CDF using a simple table.

This technique has a good performance both in terms of memory use and speed, as it takes advantage of parallelization. The procedure to generate the table is as follows:

1. The starting point is the size distribution of particles in the soot generated by the combustion of a given material. In our case, only the particle radius and the relative concentration of particles of that size are needed.
2. Next, the relative concentrations are accumulated and normalized, that is, the CDF is computed from 0 to 1. That way, for instance, if the smallest particles –radius r_0 – have a relative concentration of 8%, an interval ranging from 0 to 0.08 is assigned to them.
3. For the next particle in size, for instance radius r_1 and relative concentration 14%, the interval ranging from 0.08 to 0.22 is assigned.
4. The procedure is repeated until all the particle sizes and their relative weight have been computed (the last range will end in 1).

Using a uniform variable random generator (in the interval $[0, 1]$), it is easy to see which particle type the photon bundle is about to interact with.

In addition, for each type of particle of soot there will be a detailed table containing its scattering profile (σ in Equation 5.9).

It is important to remark the similarity of this approach to ray-tracing, since the incident signal will be modeled as a ray (in this model a “bundle” of photons). Again, the method described here differs from ray-tracing in that the ray leaving the emitter will not be divided into “child-rays”; instead, it will be “monolithic” from the emitter to its absorption, detection, etc. The remaining amount of power and its relative importance will be accounted for using statistics, which will deflect, attenuate, etc. the ray in question. The specific process is explained in section 5.5.

5.4. Geometrical model: simulation environment

In order to make a computational feasible model, it is necessary to limit the virtual space of the experiment and thus define boundaries for the simulation environment, emitter, receiver (sensor) and obstacles that photon bundles may find in their way. These constraints will be written in the corresponding configuration files.

A general scheme of the proposed setup is depicted in Figure 5.4. It comprises the following elements:

- Space.
- Emitter and Receiver.
- Object or obstacles.

Fig. 5.3.: Method used to obtain the concrete particle encountered by the photon bundle in its random walk. It outputs the particle type (radius, depicted as ' r_3 ' here) from a uniform random variable distribution and the CDF corresponding to the particle size distribution of the material being burnt.

Fig. 5.4.: Example setup proposed.

Fig. 5.5.: System of reference and definition of space geometry.

5.4.1. Space geometry

The space is the virtual environment where the simulation takes place. It defines a limit for photon bundles in an attempt to discard those that travel too far away from the line emitter–object–receiver. The space is then defined as a 6-tuple comprising the coordinates for the limits in the x –, y – and z –axis. The data is contained within a text file.

Points within this space definition meet the following statement²:

$$x_0 \leq x \leq x_1 \wedge y_0 \leq y \leq y_1 \wedge z_0 \leq z \leq z_1 \quad (5.10)$$

The system of reference and the space geometry are depicted in Figure 5.5. In the simulations proposed in this thesis, the space will be two orders of magnitude bigger than the emitter or the sensor in every direction to ensure enough room for interaction between the incoming radiation and the medium (2m for a emitter/sensor of about 1E-2m).

5.4.2. Emitter and Receiver (sensor) geometry

The source/emitter –and, too, the sensor/receiver– are modeled in a first version as a 2D planar array of pixels. The parameters needed are therefore:

- The number of pixels in the “horizontal” direction and their size (n_x, s_x).
- The number of pixels and pixel size in the “vertical” direction (n_y, s_y).
- The next three parameters account for the relative tilt of the plane and are expressed in terms of the associated normal vector of the planar array $\mathbf{v}_n$: (v_{nx}, v_{ny}, v_{nz}).
- The three last parameters (P_x, P_y, P_z) let the user define the center point of

² $\wedge$ = AND

Fig. 5.6.: Definition of source/emitter and sensor/receiver geometry parameters for a planar array in the $z = 0$ plane.

the planar array. This point and the associated normal vector of the plane define uniquely the plane where the planar array resides.

A simple sketch is given in Figure 5.6.

It is therefore possible to model many different setups using a simple set of parameters, from the simplest one where both the emitter and receiver are centered in the $z = 0$ plane to more complicated configurations with relative angles and offsets between the source and the receiver. It would be possible to define more complicated geometries for the sensor or emitter elements taking into account the effect of, for instance, lenses and other elements. This would only require minor adaptations of the source code of the model. The model only needs to locate the point of start, direction of every single emitter element (pixel) and the area occupied by the sensing device; all that in order to account for individual detections of photon bundles at each one of the sensing elements (pixels).

Typical values for the sensor and emitter array are 320×240 elements of $30 \mu m$ in both x and y directions, contained within the $z = 0$ plane and centered. As a first approximation, the sensor can be thought of being coincident with the source and therefore the emitter geometry file can be equal to the receiver geometry file.

It is necessary to state the relationship between a certain pixel (n_i, m_i) in the planar array and its corresponding point (x, y) in space:

$$(n_i, m_i) \Big|_{\substack{n_i=0 \dots n_x \\ m_i=0 \dots n_y}} = \left[\frac{(x_1 - x_0 - n_x s_x)}{2} + \frac{s_x}{2} + n_i s_x, \frac{(y_1 - y_0 - n_y s_y)}{2} + \frac{s_y}{2} + m_i s_y \right] \quad (5.11)$$

The previous expression is valid if the emitter/receiver array is planar and centered in the $z = 0$ plane. For the general case (see Figure 5.7), a more complicated expression can be derived using the next procedure:

1. Using the associated normal vector of the plane and the middle point pro-

Fig. 5.7.: General case definition of source/emitter and sensor/receiver geometry.

vided, compute the plane containing the emitter/sensor (and the parallelogram resulting from its intersection with the simulation space).

2. Using the middle point and the size of the pixel elements of the planar array, compute the limit points of the parallelogram.
3. From there, derive the limits and location of every pixel element in the array.

5.4.3. Object geometry

The geometry and properties of the objects (or obstacles) is the most diverse and hence difficult element to model. In the simplest case, the object will be just a wall located at $z = z_1$ (see Figure 5.4). More complicated obstacles and objects can be defined through the corresponding set of equations.

In addition to the geometry definition of the object(s) within the simulation space, it is necessary to define their basic physical properties. All that in order to model the interaction between the incident radiation and the object. The simplest approach is to consider the albedo³ of the surface. There are many studies comprising values for albedo for different surface materials, incident wavelengths and other factors such as aging or special-purpose coatings [238, 239]. For our application scope, an orientative value of 0.15 will be used for the albedo, in good agreement with values for middle-aged concrete, as seen in Figure 5.8(c).

Called hybrid reflection by some researchers [240], the measured reflected radiation is a mixture between specular (following Snell's Law) and diffuse reflection (Lambertian reflectance). The intensity at any point in the image of the surface may be expressed as

$$I = IL + IS = A \cos(\theta_s - \theta_n) + B\delta(\theta_s - 2\theta_n) \quad (5.12)$$

where IL is the Lambertian component and IS is the specular component. A and B are the reflectance parameters, θ_n the angle with the associated vector of the sur-

³The albedo is the fraction of the incident radiation that is reflected from the surface; see [238] for a more complete description.

Fig. 5.8.: Albedo example values for a specific concrete sample at different wavelengths and hybrid reflectance as a function of the angle.

face and θ_s the source direction. The reflectance parameters must be obtained experimentally although there have been advances in reflectance models for rough surfaces [241]. Here, the surfaces will be considered Lambertian and thus the reflectance approximated by the diffuse reflectance. It is not possible to approximate the contribution of the specular term (factor B) in general. See Figure 5.8.

5.4.4. Coordinate system and bundle propagation

The model proposed combines two coordinate systems: cartesian and spherical. Each of them is best suited for certain geometries. On the one hand, planar arrays for emitter/receivers or the parallelepiped-shaped simulation region are better expressed in terms of cartesian coordinates. On the other hand, the particle scattering data and the change in propagation direction after particle interactions are better described using spherical coordinates. In order to take advantage of both systems, part of the computation needed is done in cartesian coordinates and part in spherical; the drawback is the amount of changes in the coordinate system the model has to make and its relative impact in the overall performance. Thus, after an interaction has taken place, the cartesian coordinates of the new unitary

direction vector (x, y, z) will be a function of (θ, ϕ) as $r = 1$ (normalized):

$$(x, y, z) = \begin{cases} x = \sin \theta'' \cos \phi'' \\ y = \sin \theta'' \sin \phi'' \\ z = \cos \theta'' \end{cases} \quad (5.13)$$

where

$$\theta'' = \theta + \theta' = \arccos z + \theta' \quad (5.14)$$

$$\phi'' = \phi + \phi' = \arctan(y/x) + \phi' \quad (5.15)$$

being ϕ' a uniform random variable in the interval $[0, 360)$ and θ' the angle resulting from the interaction between the incident radiation and the matter. Expressed in mathematical terms:

$$(x, y, z) \Rightarrow \theta, \phi \rightsquigarrow \begin{cases} \theta'' = \theta + \theta' = \arccos z + \theta' \\ \phi'' = \phi + \phi' = \arctan(y/x) + \phi' \end{cases} \Rightarrow (x'', y'', z'') \quad (5.16)$$

The location, propagation direction and the actual point where the interaction between the incident radiation and the smoke particles or objects occur are tracked using cartesian coordinates. Spherical coordinates are reserved for the interactions themselves: Figure 5.9 shows the correspondence between different points and vectors in cartesian and spherical coordinates. Scattering data assumes that the radiation comes in the z -axis direction, which is equivalent to rotating the vector representing the current direction $(x, y, z) \propto$ degrees around the z -axis and β degrees around the x -axis. These rotations are represented in the figure as $x_1 - y_1 - z_1$ and $x_2 - y_2 - z_2$. The result of the interaction with the next particle is another rotation of angles γ and δ which in the end corresponds to the normalized output direction (x'', y'', z'') .

5.5. Propagation algorithm

The algorithm works in three main steps as follows (pseudocode is available in Figure 5.10):

1. **Initial step:** The outgoing photon bundle emerges from a particular pixel in the positive z semispace, while the receiver is initialized to zero.
2. **Propagation:**
 - The actual (k -th) step is computed ($w^k = -\bar{\Lambda} \log(U^k)$) and saved⁴. It corresponds to the realization of an exponential random variate with $\bar{\Lambda}$ mean.

⁴A simple, yet effective way of introducing **time resolution** into this Monte Carlo simulation is to accumulate every step length, see section 6.2.1. In the end, when a photon bundle reaches the sensing element it is possible to assign it a timestamp taking into account the sum of the steps (distance traveled) and the propagation speed (speed of light).

Fig. 5.9.: Relationship between cartesian and spherical coordinates in the proposed model.

```

init_model(geometry, optics, physical);
bundle_alive = true;
WHILE bundle_alive DO
    compute_step();
    CASE interaction IN
        reach_object{
            update_bundle_direction;
            update_bundle_power;
        }
        reach_sensor{
            save_sensor_pixel_data;
            bundle_alive = false;
        }
        reach_space_limit{
            bundle_alive = false;
        }
        default{
            interact_with_particle{
                update_bundle_direction;
                update_bundle_power;
            }
        }
    END_CASE;
END_WHILE;

```

Fig. 5.10.: Simplified model pseudocode.

- Using the actual direction of propagation and the actual step, the point reached by the wave is computed:

$$\begin{aligned} x^{k+1} &= x^k + w^k \sin(\theta^k) \cos(\phi^k) \\ y^{k+1} &= y^k + w^k \sin(\theta^k) \sin(\phi^k) \\ z^{k+1} &= z^k + w^k \cos(\theta^k) \end{aligned} \quad (5.17)$$

The following cases may be met:

- If $z \geq \rho$, being ρ the position of the intercepting surface⁵, the walk is truncated and the photon bundle is scattered back using the properties of the solid surface. That is:

$$w^k = \begin{cases} \rho - (z^k / \cos \theta^k), & \text{if } z^k + w^k \cos \theta^k \geq \rho \\ w^k, & \text{otherwise} \end{cases} \quad (5.18)$$

where z^k is the value of z in the k -th step.

In this case, only photon bundles backscattered are further propagated, the rest are considered to be absorbed.

- If the photon bundle reaches back the receiver after being intercepted by a surface in $z = \rho$, the corresponding pixel is incremented and the photon bundle ends its trip.
 - Else, the photon bundle has to interact with a particle. The interaction is described in section 5.3.2 (scattering) and 5.5.1 (power considerations).
- This step is repeated until all the photon bundles disappear (they are either absorbed, reach the sensing surface or go out of the workspace).
3. **Final step:** The aggregated response from all photon bundles at the sensing surface is computed, normalized and further processed. An image can be generated from the raw data either in greyscale or false colors (see Section 6.5.1 for more information on visualizing the results). The raw data is saved for further, finer computations with larger N (number of runs).

5.5.1. Power, absorption and free-space propagation

An important issue when it comes to modelling wave propagation is power, and as bytopics, absorption by particulate and free-space propagation. In this model, a photon bundle will be travelling from one particle to another monolithically. This means that it will change its direction without breaking into subbundles according to a certain scattering profile once it reaches a particle: it is left to the

⁵The particular case where z is the direction of propagation and $z = \rho$ is the equation of the intercepting surface is considered here.

power of statistics and big numbers combined in the Monte Carlo method to account for the combined effect of subsequent bundles. The added effect will reflect particle's scattering profiles.

This rather simple approximation has certain complications when it comes to the treatment of intensity or power associated with the propagating bundle, as the model is implicitly mixing to certain extent radiation models from wave theory and quantum physics. In the following paragraphs I will try to explain the fundamentals of the implementation of these concepts in the model.

The energy radiated on the particle is either scattered or absorbed in order to meet the energy conservation principle:

$$Q_{\text{ext}} = Q_{\text{sca}} + Q_{\text{abs}} \quad (5.19)$$

where Q_{ext} is the extinction efficiency, Q_{sca} the scattering efficiency and Q_{abs} the absorption efficiency, with

$$Q_i = \frac{\sigma_i}{\pi a^2} \quad (5.20)$$

where $i = \text{ext, sca, abs}$; a is the effective radius of the particle and σ the particle cross-section, yielding the equivalent expression:

$$\sigma_{\text{ext}} = \sigma_{\text{sca}} + \sigma_{\text{abs}} \quad (5.21)$$

Using the code by Scott Prahl [113], which is based on the original code by Wiscombe [242], it is possible to obtain the scattered intensity in the different directions. An analysis of the data provided by the software and its application is done next. In fact, data corresponding to the following expression (X is the size parameter⁶) is obtained with that code:

$$I = \frac{|S_1|^2 + |S_2|^2}{2\pi X^2 Q_{\text{sca}}} \quad (5.22)$$

S_1 and S_2 are the scattering amplitudes defined by the Lorenz-Mie theory [112] as treated by Bohren and Huffman [194].

By definition we have:

$$\int I_{\text{sca}} dA = P_{\text{sca}} \quad (5.23)$$

Besides, there is a statement concerning those values: *"The second column is normalized so that the integral of it over 4π steradians will be unity"*. Therefore,

$$\int_{\phi=0}^{2\pi} \int_{\theta=0}^{\pi} \frac{|S_1|^2 + |S_2|^2}{2\pi X^2 Q_{\text{sca}}} \sin \theta d\theta d\phi = 1 \quad (5.24)$$

⁶There seems to be a typo in the output of the code by Scott Prahl, as the second column corresponds to *"The average of the 3rd & 4th columns is the second"*). There should be a 2 in the denominator –missing in the output file–.

That is, the total scattered power is normalized in the code used. It is interesting to verify this extent: considering that the radiated intensity is constant for all ϕ we have that

$$2\pi \int_{\theta=0}^{\pi} \frac{|S_1|^2 + |S_2|^2}{2\pi X^2 Q_{sca}} \sin \theta d\theta = 1 \quad (5.25)$$

Then, breaking up the integral into intervals:

$$\begin{aligned} 1 = 2\pi & \left[\int_{\theta=0}^{\frac{\pi}{180}} I_0 \sin \theta d\theta + \int_{\theta=\frac{\pi}{180}}^{\frac{2\pi}{180}} I_1 \sin \theta d\theta + \dots + \right. \\ & \left. + \int_{\theta=\frac{178\pi}{180}}^{\frac{179\pi}{180}} I_{178} \sin \theta d\theta + \int_{\theta=\frac{179\pi}{180}}^{\pi} I_{179} \sin \theta d\theta \right] = \end{aligned} \quad (5.26)$$

As $I_0 \dots I_{179}$ are constant in the interval considered:

$$\begin{aligned} = 2\pi & \left[I_0 \int_{\theta=0}^{\frac{\pi}{180}} \sin \theta d\theta + I_1 \int_{\theta=\frac{\pi}{180}}^{\frac{2\pi}{180}} \sin \theta d\theta + \dots + \right. \\ & \left. + I_{178} \int_{\theta=\frac{178\pi}{180}}^{\frac{179\pi}{180}} \sin \theta d\theta + I_{179} \int_{\theta=\frac{179\pi}{180}}^{\pi} \sin \theta d\theta \right] = \end{aligned} \quad (5.27)$$

Integrating gives:

$$\begin{aligned} = 2\pi & \left[I_0 \left(-\cos \frac{\pi}{180} + \cos 0 \right) + I_1 \left(-\cos \frac{2\pi}{180} + \cos \frac{\pi}{180} \right) + \dots + \right. \\ & \left. + I_{178} \left(-\cos \frac{179\pi}{180} + \cos \frac{178\pi}{180} \right) + I_{179} \left(-\cos \pi + \cos \frac{179\pi}{180} \right) \right] = 1 \end{aligned} \quad (5.28)$$

Which is true for the data obtained using the code: after computing the previous expression for 500 angle intervals we obtain unity with an error lower than $\pm 0.02\%$ (attributable to round-off errors).

In addition, it is known that the scattered field $\vec{E}_s$ can be expressed in terms of $E_{s\theta}$ and $E_{s\phi}$ (k is the wavenumber) with:

$$\begin{aligned} E_{s\theta} &= \frac{e^{jkr}}{-jkr} \cos \phi S_2(\cos \theta) \\ E_{s\phi} &= \frac{e^{jkr}}{jkr} \sin \phi S_1(\cos \theta) \end{aligned} \quad (5.29)$$

Therefore, the magnitude of the scattered field will be

$$|E_s| = \sqrt{|E_{s\theta}|^2 + |E_{s\phi}|^2} \quad (5.30)$$

so those values obtained are proportional to the scattered intensity in that direction.

Recalling the energy conservation principle (being P_i the incident power and P_{sca} and P_{abs} the scattered and absorbed power respectively) we can write:

$$P_i = P_{sca} + P_{abs} \quad (5.31)$$

Or in terms of cross-sections:

$$P_{sca} = P_i \left(1 - \frac{\sigma_{abs}}{\sigma_{ext}}\right) = P_i \frac{\sigma_{sca}}{\sigma_{ext}} \quad (5.32)$$

So the total output power emanating from a particle would be

$$P_{out} = P_{sca} = \int_{\alpha_0}^{\alpha_1} I_{sca} dA \quad (5.33)$$

And the output power emanating from a particle in a certain direction given by the angle interval in the data obtained from Prahl's code is:

$$P_{out,dir} = P_i \frac{\sigma_{sca}}{\sigma_{ext}} \int_{\alpha_0}^{\alpha_1} I dA \Big|_N \quad (5.34)$$

In the previous equation, $\int_{\alpha_0}^{\alpha_1} I dA \Big|_N$ can be seen as a dimension-less factor because it is normalized to unity for 4π steradians and only accounts for the fraction of total power radiated in that direction (considered as a solid angle).

Although not crucial given the short distances covered by the model, the effect of radiation power dispersion due to distance can be included as well by means of a distance factor and recalling that the radiated power decreases with r^{-2} , where r is the distance traveled by the radiation (see section 3.2.2). In this case, if the relative superposition of the areas of the radiating particle and the particle receiving the radiation is not considered, the total scattered power averaged per unit area that reaches a particle $P'_{i,n}$ can be expressed as:

$$P'_{i,n} = P_{out} \frac{1}{4\pi r^2} \quad (5.35)$$

However, if only the power emitted in a certain spherical cap is considered $P_{out,dir}$, the previous expression becomes (see Figure 5.11):

$$P'_{i,n} = P_{out,dir} \frac{1}{r^2 \int_{\alpha_0}^{\alpha_1} dA} \quad (5.36)$$

The total averaged power illuminating the particle will be then (being σ'_{ext} the extinction cross-section of the particle where the radiation is incoming):

$$P'_i = P'_{i,n} \sigma'_{ext} = P_{out} \frac{\sigma'_{ext}}{4\pi r^2} \quad (5.37)$$

Fig. 5.11.: Radiated average intensity in the sphere vs. radiated average intensity in a certain spherical cap.

Considering only the power illuminating the particle coming in a certain direction:

$$\begin{aligned} P'_i &= P'_{i,n} \sigma'_{ext} = P_{out,dir} \frac{\sigma'_{ext}}{r^2 \int_{\alpha_0}^{\alpha_1} dA} \\ &= P_i \frac{\sigma_{sca}}{\sigma_{ext}} \int_{\alpha_0}^{\alpha_1} I dA \Big|_N \frac{\sigma'_{ext}}{r^2 \int_{\alpha_0}^{\alpha_1} dA} \end{aligned} \quad (5.38)$$

Ordering terms:

$$P'_i = P_i \frac{\sigma_{sca}}{\sigma_{ext}} \frac{\sigma'_{ext}}{r^2 \int_{\alpha_0}^{\alpha_1} dA} \int_{\alpha_0}^{\alpha_1} I dA \Big|_N \quad (5.39)$$

Provided that in this model I is a constant in the interval considered, $I = I_{\alpha_0, \alpha_1}$, it is possible to simplify equation 5.38:

$$P'_i = P_i \frac{\sigma_{sca}}{\sigma_{ext}} \frac{\sigma'_{ext}}{r^2} I_{\alpha_0, \alpha_1} \Big|_N \quad (5.40)$$

In order to state the effect due to absorption in the values provided by the data obtained using the code in [113], several operations have to be conducted⁷:

1. Normalize for unity

$$\sum_{\forall \alpha_i} I_{\alpha_0, \alpha_1}$$

(I is constant but different in each interval).

⁷There is no difference between the values in column two obtained directly from the code that are divided by $2\pi X^2 Q_{sca}$ and the values corresponding to $|S_1|^2 + |S_2|^2$ and normalized to one since $2\pi X^2 Q_{sca}$ is a constant. There is no point in performing the operation and therefore it has not been included in the list of operations to be done.

Fig. 5.12.: Analytical computation of the transmitted power using the procedure in our model. Simplification of the σ_{ext} factor for subsequent particle interactions. [P_i is the input power, σ_{ext} the extinction cross-section, σ_{abs} the scattering cross-section and I_N the normalized intensity weight factor (for particle 1). r is the distance between particle 1 and 2, and σ'_{ext} the extinction cross-section, σ'_{abs} the scattering cross-section and I'_N the normalized intensity weight factor (for particle 2)].

2. Multiply all the values times σ_{sca} . σ_{ext} will be simplified out after interaction with the particle as shown in Figure 5.12.

Once obtained, the results will be stored for their computation and conversion to the CDF format (see section 5.3.2), which is the one used in the implementation.

5.6. Simulation setup

A number of parameters have to be defined to analyze different smoke scenarios. Several have been considered:

- **Particle size distribution:** Size and relative concentration of particles for different materials have been studied and computed using the data and procedures in section 4.1.3.2. The incident bundle will interact with particles of different sizes depending on the material being burnt and the conditions of the fire (flaming, nonflaming, etc.).
- **Density of particles:** Using data from [243] and [244], the number of particles per unit volume is retrieved. The volume concentration is then computed for the different types of smoke materials and situations (flaming and nonflaming) using the particle size distributions: radius and relative concentration.

In this first version of the model, only uniform distributions of particles (with arbitrary scattering profiles and size concentrations) will be considered. Minor changes in the algorithm and the code would suffice to open the model to the possibility of working with customizable nonuniform at-

Tab. 5.1.: Operating wavelengths of state of the art solid state lasers and the corresponding wavelength chosen for simulation (compiled using the data in 3.5).

Semiconductor	Operating λ (nm)	Value of λ for simulation (nm)
InGaN	370-493	400
GaN	515-520	515
InGaAlP	630-685	650
GaAlAs	750-850	800
InGaAs	904-1065	1000
"	1270-1330	-
"	1430-1570	1500
AlGaIn/AsPb	1870-2200	2000
Pb salts	3300-27000	3500

mospheres.

- **Mean free path (Λ or MFP):** Using the values of the volume concentration of particles and the particle size distributions obtained above, together with Equation 5.4, it is possible to derive the value of the MFP in microns. Three cases have been considered:
 1. *Best-case* - Λ_{MAX} ("thin" medium). Implies a higher MFP. The value of the mean free path is computed using the diameter of the biggest particle in the smoke and the lowest scattering efficiency of all particles in the smoke for that particular wavelength (λ) and material.
 2. *Worst-case* - Λ_{min} ("thick" medium). Implies a lower MFP. In this case, the diameter of the smaller particle and the highest scattering efficiency is used.
 3. *Average case*. Λ_{avg} is computed using the pondered value of the particle diameter and the scattering efficiency for the particular size distribution and burning conditions (material, flaming or nonflaming, etc.).

These three cases should provide with a scope wide enough to obtain data well correlated with reality. They can also be of help proposing setups for the design of real devices.

- **Wavelength ranges (λ):** Several representative wavelengths (see Table 5.1) have been chosen ranging from 400nm to 3500nm, taking into account the availability of solid-state lasers and recalling that the main aim of this work is to create a development framework for real-world applications.
- **Temperature:** The possible variations in behavior due to the presence of air and other gases at different temperatures has been accounted for as well. This has been done computing the refraction indices of air at different temperatures that can be found in compartment fires (50, 150, 300, 600 and 900°C) using the Ciddor equation [245] or the Edlén equation [246], both

available as software online [247].

- **Phase function:** it is computed for every particle type considered for all the cases considered in the simulation. The code used for this task is from Scott Prahl [113], which is based on the original Fortran77 code by Wiscombe [242]. Besides, the software *mieplot* by Philip Laven [248] has been used to compute and display phase functions, as well as for other tasks (computation for different temperatures, simulation of particle size distributions, etc.).

However, it is not the phase function what is needed to feed the model for the simulations, but the CDF resulting from the phase function, which is computed following the same method as the one explained above for particle size distributions.

Table 5.2 shows the size factor of each particle type and incident wavelength considered for the materials studied in section 4.1.3. Larger values of the size factor correspond to more directive scattering patterns (as depicted in Figures 3.8 or 3.9). The cells have been colored in order to stress and ease the visualization of the data therein. Three color groups have been made: cases with particle size parameter less than 3, between 3 and 6 and greater than 6. This way it is possible to see the agreement between these values and the results obtained by the simulations for different cases and compare them to the behavior predicted by the Mie theory as a first concept check of the model.

5.7. Simulation results

In order to gather information about the performance and validity of the proposed model itself, several software tests were conducted. Each test is a series of 100 runs of the model for a certain set of conditions (setup). A total of 843 distinct tests were conducted. The first 228 were carried out several times to check the consistency of the Monte Carlo method implemented. The rest (615) were conducted only once for each setup of the model.

Each setup is made defining a number of parameters:

- *Material:* fir (flaming), fir (nonflaming), oil, polyurethane, PVC (flaming), PVC (nonflaming), wood.
- *Temperature:* 50°C, 150°C, 300°C, 600°C, 900°C.
- *Incident wavelength* (μm): 0.4, 0.515, 0.650, 0.800, 1.000, 1.500, 2.000, 3.500.
- *Mean free path:* worst-case, average case, best-case (different for each material and determined by equation 5.4).
- *Geometrical setup:*
 - *Space environment:* a cube of 2m side has been considered.
 - *Emitter and receiver* will be coincident, each will form an array of 320x240

Tab. 5.2.: Size factor depending on the burning material and smoke particle size (λ in μm). Three color groups have been made: cases with particle size parameter less than 3, between 3 and 6 and greater than 6.

Material	Particle radius	Relative frequency (%)	$\lambda=0.4$	$\lambda=0.515$	$\lambda=0.65$	$\lambda=0.8$	$\lambda=1.0$	$\lambda=1.5$	$\lambda=2.0$	$\lambda=3.5$
Firflam	0.225	48.10	3.53	2.75	2.17	1.77	1.41	0.94	0.71	0.40
Firflam	0.335	19.04	5.26	4.09	3.24	2.63	2.10	1.40	1.05	0.60
Firflam	0.600	21.04	9.42	7.32	5.80	4.71	3.77	2.51	1.88	1.08
Firflam	1.100	5.01	17.28	13.42	10.63	8.64	6.91	4.61	3.46	1.97
Firflam	1.750	4.01	27.49	21.35	16.92	13.74	11.00	7.33	5.50	3.14
Firflam	2.450	2.81	38.48	29.89	23.68	19.24	15.39	10.26	7.70	4.40
Firnonflam	0.225	10.02	3.53	2.75	2.17	1.77	1.41	0.94	0.71	0.40
Firnonflam	0.335	25.05	5.26	4.09	3.24	2.63	2.10	1.40	1.05	0.60
Firnonflam	0.600	25.05	9.42	7.32	5.80	4.71	3.77	2.51	1.88	1.08
Firnonflam	1.100	22.04	17.28	13.42	10.63	8.64	6.91	4.61	3.46	1.97
Firnonflam	1.750	13.03	27.49	21.35	16.92	13.74	11.00	7.33	5.50	3.14
Firnonflam	2.450	4.81	38.48	29.89	23.68	19.24	15.39	10.26	7.70	4.40
Oil	0.260	48.19	4.08	3.17	2.51	2.04	1.63	1.09	0.82	0.47
Oil	0.465	12.05	7.30	5.67	4.49	3.65	2.92	1.95	1.46	0.83
Oil	0.775	9.64	12.17	9.46	7.49	6.09	4.87	3.25	2.43	1.39
Oil	1.750	12.05	27.49	21.35	16.92	13.74	11.00	7.33	5.50	3.14
Oil	3.000	4.82	47.12	36.60	29.00	23.56	18.85	12.57	9.42	5.39
Oil	4.900	13.25	76.97	59.78	47.37	38.48	30.79	20.53	15.39	8.80
Oil	7.400	0.00	116.24	90.28	71.53	58.12	46.50	31.00	23.25	13.28
Oil	10.650	0.00	167.29	129.93	102.95	83.64	66.92	44.61	33.46	19.12
Polyurethane	0.225	26.88	3.53	2.75	2.17	1.77	1.41	0.94	0.71	0.40
Polyurethane	0.335	18.28	5.26	4.09	3.24	2.63	2.10	1.40	1.05	0.60
Polyurethane	0.600	17.20	9.42	7.32	5.80	4.71	3.77	2.51	1.88	1.08
Polyurethane	1.100	23.66	17.28	13.42	10.63	8.64	6.91	4.61	3.46	1.97
Polyurethane	1.750	13.98	27.49	21.35	16.92	13.74	11.00	7.33	5.50	3.14
PVCflam	0.225	48.39	3.53	2.75	2.17	1.77	1.41	0.94	0.71	0.40
PVCflam	0.335	19.15	5.26	4.09	3.24	2.63	2.10	1.40	1.05	0.60
PVCflam	0.600	25.20	9.42	7.32	5.80	4.71	3.77	2.51	1.88	1.08
PVCflam	1.100	6.05	17.28	13.42	10.63	8.64	6.91	4.61	3.46	1.97
PVCflam	1.750	1.21	27.49	21.35	16.92	13.74	11.00	7.33	5.50	3.14
PVCnonflam	0.225	25.25	3.53	2.75	2.17	1.77	1.41	0.94	0.71	0.40
PVCnonflam	0.335	15.15	5.26	4.09	3.24	2.63	2.10	1.40	1.05	0.60
PVCnonflam	0.600	27.27	9.42	7.32	5.80	4.71	3.77	2.51	1.88	1.08
PVCnonflam	1.100	25.25	17.28	13.42	10.63	8.64	6.91	4.61	3.46	1.97
PVCnonflam	1.750	7.07	27.49	21.35	16.92	13.74	11.00	7.33	5.50	3.14
Wood	0.028	0.00	0.44	0.34	0.27	0.22	0.18	0.12	0.09	0.05
Wood	0.050	0.16	0.79	0.61	0.48	0.39	0.31	0.21	0.16	0.09
Wood	0.090	0.39	1.41	1.10	0.87	0.71	0.57	0.38	0.28	0.16
Wood	0.160	1.32	2.51	1.95	1.55	1.26	1.01	0.67	0.50	0.29
Wood	0.280	4.97	4.40	3.42	2.71	2.20	1.76	1.17	0.88	0.50
Wood	0.500	17.08	7.85	6.10	4.83	3.93	3.14	2.09	1.57	0.90
Wood	0.900	38.51	14.14	10.98	8.70	7.07	5.65	3.77	2.83	1.62
Wood	1.600	23.60	25.13	19.52	15.47	12.57	10.05	6.70	5.03	2.87
Wood	2.800	13.20	43.98	34.16	27.07	21.99	17.59	11.73	8.80	5.03
Wood	5.000	0.78	78.54	61.00	48.33	39.27	31.42	20.94	15.71	8.98

square $30\mu\text{m}$ -sided-elements centered at $(1, 1, 0)\text{m}$ (the center of a side of the space cube).

- *Object*: a concrete wall with albedo 0.15, coincident with the side of the space cube located at $z = 2\text{m}$. It is important to recall that arbitrary objects can be placed in the simulation environment provided that their geometries, location and optical properties are fed into the model.
- *Emitter power and receiver sensitivity*: the noise floor is set to -60dBm arbitrarily, as the only limitation of the model is due to the number representation range in the computer. The receiver is able to detect all photon bundles with power levels over the noise floor. The per-pixel emitted power is set to 1dBm . This power has been chosen very high on purpose and will have its implications: the importance of attenuation will be underweighted and that of scattering overweighted.

A total of 7.68 mega photon bundles were therefore simulated for each simulation setup ($320 \times 240 \times 100$). The data provided for each setup was then reduced and weighed (%) in order to track the final destinations (termination codes in the software) of the corresponding photon bundles:

1. *Attenuated*: power falls below detection level before reaching the sensor.
2. *Out of sensor*: the photon bundle reaches the emitter (sensor) plane, but the received bundle falls out of the sensor area. It may be related to backscattering at early stages of the propagation.
3. *Absorbed*: the bundle reached the object (the concrete wall with albedo 0.15) and was absorbed.
4. *Out of space*: the photon bundle is scattered away out of the simulation space.
5. *Successful detection*: the bundle reached the sensor and excited the corresponding array element (pixel).

5.7.1. Self-consistency checks

In a first moment, only statistical consistency as long as some proof-of-concept simulations and checks were conducted with the geometrical setup in Figure 5.4. Please refer to Chapter 7 for more information about validation experiments.

The first 228 cases were run up to 6 times each in order to assess the statistical consistency of the model. The final destinations of the bundles were considered: the relative number (in %) of attenuated, out of sensor, absorbed, etc. photon bundles was computed and used as the initial data (absolute values). Thus, for each of the 228 cases, the arithmetic average for the final destination of each bundle was computed, as well as the absolute data scatter (absolute value of the difference between the average and the absolute values –for each termination code–).

Fig. 5.13.: Data scatter plots showing self-consistence of the model (% of photon bundles with a certain termination code).

The relative data scatter was computed as well, see Figure 5.13.

In Figure 5.13(a), the relative data scatter vs. the absolute value of the particular termination code is plotted. There it is possible to see relative data scatters in excess of 100% for absolute values of less than 5E-5%, which mainly correspond to “out of space” exit codes. These big variances are related to residual values (few bundles end with that termination code and therefore an insignificant variation of less than 10 out of millions of bundles may mean relative differences well over 100%). Remarkably, relative data scatter falls under 1% for absolute values over 0.1%.

Plotting the absolute data scatter vs. the relative data scatter (see Figure 5.13(b)), it is possible to see that for an absolute data scatter of over 0.001, the relative data scatter falls below 1%. Again, scatters over 1% happen for very low occurring (rare) events.

The main result that can be extracted is that the model is statistically consistent and that the setups and simulations run converge rapidly, enabling the extraction of conclusions from the available data.

5.7.2. Analysis of the simulations and potential of the model

In order to illustrate the potential of the proposed model and as a proof-of-concept, several plots have been included. The data obtained makes it possible to analyze signal propagation from a number of perspectives only by changing the data supplied to the model, device properties or other contour conditions. The model can give a huge amount of data from each photon bundle, which can be aggregated in order to draw qualitative as well as quantitative conclusions.

For instance, Figures 5.14 and 5.15 show that temperature dependence is negligible for a variety of materials and wavelengths, taking into account the particular conditions of the setups (uniform temperature and atmosphere, etc.).

It would be possible to compare the behavior of wave propagation for several fire types (represented here by the burning material) and a number of wavelengths in order to gain insight into the performance of the system for certain setup. Plots in Figures 5.16, 5.17 and 5.18 gather the results for fir (flaming vs. nonflaming), PVC (flaming vs. nonflaming), and oil vs. wood at 300°C. It is important to remark the dependence of the results with the incident wavelength, which is in good agreement with the Mie theory.

For all the simulated materials, the prevalent mechanism of photon bundle termination is absorption at the object for wavelengths under 1.0μm, while attenuation or even backscattering are dominant at higher wavelengths. This *a priori* surprising result can be easily explained when considering the high power emitted by each pixel (1dBm) and the detector sensitivity (-60dBm) which, as said before, underweights the relative importance of attenuation as an extinction mechanism

Fig. 5.14.: Dependency on the temperature of the aggregated photon bundles terminated with codes "Attenuation" and "Out of sensor" for different materials.

(a) Absorption

(b) Out of space

Fig. 5.15.: Dependency on the temperature of the aggregated photon bundles terminated with codes “Absorption” and “Out of space” for different materials.

(a) Fir (flaming)

(b) Fir (non flaming)

Fig. 5.16.: Model termination codes for the aggregated photon bundles for flaming fir and non flaming fir at 300°C.

(a) PVC (flaming)

(b) PVC (nonflaming)

Fig. 5.17.: Model termination codes for the aggregated photon bundles for flaming PVC and non flaming PVC at 300°C.

(a) Oil

(b) Wood

Fig. 5.18.: Model termination codes for the aggregated photon bundles for oil and wood at 300°C.

for lower wavelengths and stresses the importance of scattering and absorption at the concrete wall. This tendency is replicated in lighter smoke scenarios (corresponding average or best-case simulations, not shown in the figures).

5.8. Concluding remarks

In this chapter, a framework model to simulate the propagation of electromagnetic signals has been presented. Its design has been made with modularity and generality in mind. This way, despite being primarily intended for smoke and fire scenarios, it is easily configurable or adaptable to be used in other cases as well. The model is a bridge between models studying particle-filled atmospheres as a macroscopic fluid and those of particle Physics studying the interactions between incident signals and individual particles. An analytical derivation of the equations and expressions coded in the model has been presented as well giving birth to a framework model no longer tied to a particular case (underwater, search-and-rescue operations, etc.).

Simulation results from self-consistency software tests, as well as proof-of-concept results have been shown and discussed. A simple setup in which the emitter is facing a concrete wall has been simulated, although the model would show its full potential when more objects are included in the simulation chamber in a more realistic setup: the prediction of the behavior of the medium in those cases is actually the final aim of the model. The amount of data offered by the model makes it necessary to develop additional visualization tools to be able to draw relevant conclusions (see section 6.5.1). These tools take into account other information also provided by the model such as time of flight, individual sensors activated, etc. whose exploitation could be useful. Next chapter is devoted to these questions, focusing on the practical implementation of the algorithms.

6. Implementation, optimization and exploitation of the model

"Almost all quality improvement comes via simplification of design, manufacturing, processes, and procedures."

Tom Peters

In the last years, CPUs have not incremented their clock speeds significantly due to radiative and dissipative issues, among other factors. The race for speed has changed from being CPU clock-centric to novel hardware architectures featuring high degree of parallelism. In that sense, multicore CPUs and multiCPU computers have populated professional data centers and home computers alike, making it possible for developers to take advantage from these advances.

Simultaneously, the use of Graphic Processing Units (GPUs) to solve problems not explicitly related to graphics (General-Purpose GPU, or GPGPUs) has released the huge processing capabilities of the radically-parallel architectures of the GPUs for complex problems at a fraction of the cost of a traditional multi-CPU approach [249].

6.1. Related work

One of the most promising fields of use for GPGPUs is undoubtedly the simulation of physical systems –as is our case– [250, 251]: the computational power available makes it possible to obtain simulation results of complex systems from the simulation of its basic constituents. The possibility of extracting rapid or even real-time data from computer-generated simulations is very interesting, as it makes rapid prototyping and shorter times to market possible. Within that framework, performance issues are highly relevant. Research interests have evolved in the last decade, from parallel vs. serial (ie. CPU vs. GPU) comparisons of implementations to general parallelization finetuning [252, 253, 254, 255].

A performance analysis of different implementations of the model presented earlier is conducted here, complementing previous studies on memory perfor-

mance in parallel architectures [256, 257, 258]. A careful algorithm design and implementation procedure has been followed, aiming for a perfect fit to the GPU architecture in order to maximize performance.

6.2. On the model and its implementation

The model presented in chapter 5 exhibits a **high degree of parallelism** and remarkably, the different **photon bundles** (which will be implemented as threads) **do not interact with each other**. Photon interaction can be discarded as photon-photon interaction is negligible in the visible regime (where photon energies are of the order of a few eV). In addition, in classical electrodynamics, the Maxwell equations are linear and cannot describe any photon-photon interaction. Nevertheless, it is important to stress the fact. It is more a formal assessment than a scientific one, as the model is launching and following “photon bundles” in the positive z-semispace (see Section 5.2): it is possible to reduce the intensity per bundle arbitrarily by increasing the number of runs of the model for a certain illumination power.

These basic ingredients make this model a good candidate for parallelization.

Not only the GPU theoretical capabilities are important, but the set of developing tools to exploit them. The model has been implemented using Compute Unified Device Architecture (CUDA) (the parallel computing platform and programming model developed by NVIDIA to exploit their GPGPUs; extensive developer documentation is available in [259]). Figure 6.1 shows a general diagram of the algorithm implementing the model.

Two implementations, one featuring CUDA Unified Virtual Memory (UVM) and another one featuring manual optimizations have been developed and will be compared below for different simulation setups. The results will lead to a set of conclusions and practical directions to maximize performance under a real-world scenario.

6.2.1. Practical considerations regarding the implementation

As said before, the availability of affordable parallel computation has increased research interest in the area and thus rapid advances. In computer graphics, for instance, approaches similar to the one described here have been exploited to improve existing ray-tracing and scattering algorithms [260, 261].

As seen on previous sections, the method used to simulate the propagation of electromagnetic radiation through smoke-filled atmospheres has been a **time-resolved event-based Monte Carlo method**. Time resolution has been achieved recording the distance traveled by each photon bundle and recalling that the

Fig. 6.1.: Scheme of the CUDA algorithm to simulate the propagation of an electromagnetic signal through smoke or other particle-filled atmospheres.

equation of space-time for uniform linear motion with constant velocity is $s = vt$, with $v = c$ (the speed of light), s space and t time.

An important question in any method involving random numbers is the generation of those numbers, since the quality of the *Random Number Generator (RNG)* will largely impact on the final result of the simulation –biases in uniform random number generators can lead to bad results and misinterpretations of those results–. There are many papers and related work in the topic (see [262, 263] for general or Monte Carlo-related considerations or [264] for in-depth descriptions of real- vs. quasi- vs. pseudo- random number generators and their implementations)¹.

The implementation presented here relies on the built-in CUDA functions contained in the CURAND library [265]. This library provides with functions that generate both quasirandom or pseudorandom sequences. Details of the implementation of those functions with links to research papers are included in the CUDA Toolkit Documentation. In our case, the functions used are `curand_init` and `curand_uniform_double`.

The uniformly distributed random numbers are then converted to the suitable CDFs. This is done either:

1. Using the Devroye method (computation of the realization of the exponential random variable that models the step length).
2. Following the steps presented in section 5.6. These steps are followed to find out the type of particle encountered by the photon bundle and also to compute the result of the interaction between the particle and the incoming radiation.

The repetition of this process creates a truly random walk for the photon bundles.

6.2.2. Programming model: GPU and CPU data structures

Once the geometry of the model has been explained (see section 5.4), the data structures needed in the implementation become clearer and easier to understand and implement. The general idea behind the implementation of this Monte Carlo propagation model in a GPU is to speedup the simulation taking advantage of their inherent parallel architecture.

As seen in previous sections, an important advantage of this particular model is the independence of each photon bundle, that is, they do not interact or in any manner have influence on one another. This fact avoids long waits or dependence on the execution of different threads. Besides, this way there is a convenient

¹As a sidenote example of the growing importance of RNGs, the interested reader may recall the impact of the polemical publication regarding the unauditable hardware generation of random numbers in the linux kernel.

Fig. 6.2.: Buildup of threads and blocks in the GPU.

identity between threads and pixel/photon bundles (see Figure 6.2).

Any particular pixel (x, y) can be addressed by the GPU tuple $(\text{blockIdx.x} * \text{blockDim.x} + \text{threadIdx.x}, \text{blockIdx.y} * \text{blockDim.y} + \text{threadIdx.y})$. Geometrical correspondences with the GPU thread identifiers can also be done:

$$\begin{aligned} \text{pixel}_x &= P_{x_0} + (\text{blockIdx.x} \times \text{blockDim.x} + \text{threadIdx.x})s_x \\ \text{pixel}_y &= P_{y_0} + (\text{blockIdx.y} \times \text{blockDim.y} + \text{threadIdx.y})s_y \end{aligned} \quad (6.1)$$

where $P(P_{x_0}, P_{y_0}, 0)$ corresponds to the bottom left point in space for the case where the emitter/receiver is located centered in the $z = 0$ plane. Therefore,

$$\begin{aligned} P_{x_0} &= \frac{1}{2}(x_1 - x_0) - s_x \left\lceil \frac{\text{blockDim.x}}{2} \right\rceil \\ P_{y_0} &= \frac{1}{2}(y_1 - y_0) - s_y \left\lceil \frac{\text{blockDim.y}}{2} \right\rceil \end{aligned} \quad (6.2)$$

The approach presented here is memory intensive (i.e. the bottleneck of the algorithm is memory access): every thread looks up data in memory many times through its execution. Appropriate use of memory is crucial to speed things up, in particular the use of fast cache (on chip) memory [266]. Registers and shared memory, followed by constant memory is favored due to their high speeds. Data

Fig. 6.3.: "Flattening" of tables.

tables are read from disk files and stored in RAM (host) memory, which is later copied to the device (global memory). Using a collaborative approach, those tables in global memory are transferred to shared memory² and "flattened" (transformed from 3D or 2D tables to 1D tables, see Figure 6.3). Global parameters on the other hand (geometry definitions) are first transferred to device constant memory and later to registers for fastest access.

It is possible to further exploit parallelization in order to do the final table lookup for scattering data [267]: instead of conducting a binary search once the random number has been obtained from the uniform generator, n threads (n being the number of distinct particle sizes) running in parallel can find out the particle size using a simple if clause³:

```
if (random_number >= thread_number[lower_range_limit])
    and (random_number < thread_number[upper_range_limit])
{
    particle_radius = thread_number[radius]
}
```

This method is not very advantageous for low number of types of particles; in our setups this number is not larger than 10. Bigger gains can be achieved for larger datasets, which is the case for the computation of the output direction of the photon bundle once it has interacted with a certain particle.

Although this method is superior in concept, the lack of implementation of nested kernels for CUDA devices with computing capabilities ≤ 3.5 has conditioned the serial implementation of the search. Even for the serial case, several

²Despite the small amount of shared memory, the design of the tables and input parameters make it possible to fit all data in about 24KB and therefore in shared memory.

³Note that it will be necessary to add a clause for the special case: `random_number = 1.`

Fig. 6.4.: Sequential vs. Binary search: cost expressed as the mean number of iterations vs. number of elements in the dataset.

approaches can be taken. In this case, the most cost-effective ones would be sequential or binary search. As seen in Figure 6.4, sequential search is more costly than binary search if the ordered dataset has more than ≈ 17 elements. The decision is therefore clear, sequential search for the size distribution tables and binary search for the scattering tables.

6.3. Implementation finetuning for enhanced performance

Starting with CUDA6, NVIDIA released what is called “Unified Memory”, a novel memory management that hides the complexity of moving data from RAM to GPU (RAM, shared, constant or register). By doing this, the entry level to GPU programming is lowered and thus accessible to a wider audience of developers. There is the doubt, however, of whether the automatic management of GPU memory outperforms the optimizations done by hand. With this idea in mind and taking advantage of the coincident release of CUDA6 at the time, a second implementation of the model was done using CUDA6 and Unified Memory. In computation-intensive applications such as the one presented here it is worth exploring new ways of improving performance due to the high number of concurrent processes and iterations: a slight execution time reduction may mean significant time savings when considering its added effect. This is the main rea-

Fig. 6.5.: Memory hierarchy. Taken from old NVIDIA documentation.

son behind this study.

The comparison between the results obtained by the two versions are summed up and commented in section 6.4.

6.3.1. CUDA5.5

In general, there are two design paradigms that allow the use of parallelism efficiently:

- Partition the computation among the different multiprocessors equally to keep them busy (more threads with more thread blocks).
- Keep resource usage low enough so that all the threads can be active concurrently.

It is important to recall the fact that there are **three different levels of memory**; from faster to slower: registers, shared memory and device memory (texture, constant, local and global): see Figure 6.5. All models of NVIDIA GPUs at the time of writing have those types of memories, although they differ on the amount of registers or memory sizes. Here, manual optimization of the data transfers and memory assignment has been conducted as follows:

- Tables containing particle size distribution and scattering data have been moved to *shared memory*.
- Parameters and geometrical parameters corresponding to the simulation environment have been moved to *constant memory* first and then to thread registers for faster access. Every thread has to move this data from “global” constant memory to their local registers, which is the reason why this data has been located in constant memory (faster) instead of device global memory (slower).

- *Thread local memory* use has been reduced to the minimum.
- Threads do *not* access device global memory except for coalesced per-block copy of the data tables (size distribution and scattering data) to shared memory (which is done only once).
- Thread *registers* are heavily used to store all the relevant variables for the Monte Carlo model. The result is copied back to device global memory once the thread has ended and ultimately to RAM (host memory) for file output.

The two main design paradigms outlined before have been followed, with register use under 30% for 256 thread block size (25% of the maximum amount of threads per block). This has allowed high occupancy of the multiprocessors (63-100% depending on the number of types of particles considered).

6.3.2. CUDA6

An alternative implementation making use of the Unified Memory feature available in CUDA6 was also done, trying to remove any “manual” optimization thus letting CUDA manage memory assignment and data transfers between RAM (host memory) and the device. Maximum care has been put to try not to influence performance any other way. It is to remark the ease of moving a CUDA5.5 implementation to CUDA6: the code gets cleaner and easier to read and maintain, since the details of the data moves between device and host are hidden to the programmer.

6.4. Profiling and results

This section has been divided into three parts: real simulations using the setups proposed in Table 6.1 for the code versions considered (CUDA5.5, CUDA6-MAN and CUDA6-UVM), limited simulations designed to stress the effects of manual optimizations vs. CUDA automatic optimizations, and some comments on performance enhancement and cost-effectiveness from an integral point of view.

6.4.1. Case study simulations

A total set of 54 different setups were simulated: 18 for CUDA5.5, 18 for CUDA6 using the same code as for CUDA5.5 and 18 for CUDA6 using Unified Virtual Memory (UVM). The system used for the simulations was a machine running GNU/Linux 3.13.5 with an Intel i7 CPU, 8GB of RAM and a NVIDIA GT 650M GPU (NVIDIA proprietary driver, version 331.49).

Tab. 6.1.: Environment setups.

Setup #	Material	Environment	Mean free path (μm)	Particle types
1	PVC (flaming)	Ideal	62810.41	5
2	PVC (flaming)	Ideal	493816.34	5
3	PVC (nonflaming)	Ideal	17089.39	5
4	PVC (nonflaming)	Ideal	134357.00	5
5	Wood	Ideal	312.49	10
6	Wood	Ideal	2423477.32	10
7	PVC (flaming)	Albedo-only	62810.41	5
8	PVC (flaming)	Albedo-only	493816.34	5
9	PVC (nonflaming)	Albedo-only	17089.39	5
10	PVC (nonflaming)	Albedo-only	134357.00	5
11	Wood	Albedo-only	312.49	10
12	Wood	Albedo-only	2423477.32	10
13	PVC (flaming)	Realistic	62810.41	5
14	PVC (flaming)	Realistic	493816.34	5
15	PVC (nonflaming)	Realistic	17089.39	5
16	PVC (nonflaming)	Realistic	134357.00	5
17	Wood	Realistic	312.49	10
18	Wood	Realistic	2423477.32	10

The setups chosen correspond to the propagation of optical radiation at a wavelength of $0.4\mu\text{m}$ through different smoke-filled atmospheres. A summary of the most important features of the setups can be seen in Table 6.1. All of them share several parameters:

- Geometry of the simulation environment: space (cube with edge=2m), emitter and receiver (320×240 square pixels of $30\mu\text{m}$ side each) and object (wall located at $z = 2\text{m}$).
- Emitted power (pixel): 1.
- Attenuation/Detection limit: 10^{-60} .
- Object Albedo (where applicable): 0.15.
- Boundary Factor: 0.05.
- Number of Runs: 1000.

The simulated environments include three types of smoke corresponding to different materials: PVC with flame, PVC without flame and wood. Light smoke as well as heavy smoke (thus the different mean free paths) have been considered for each material. For comparison, another two sets of environments, one corresponding to ideal conditions (non-scattering atmosphere and a perfect reflecting surface) and the other to albedo-only conditions (non-scattering atmosphere but a surface with albedo assimilable to concrete) have been included as well.

Tab. 6.2.: Run times in microseconds normalized per particle interaction for CUDA5.5 and CUDA6 versions of the code. Corresponding percentage gains referred to CUDA5.5 are included.

Setup #	Material	Environment	Average number of interactions	CUDA5.5	CUDA6 MAN	CUDA6 UVM	CUDA6 MAN gain (%)	CUDA6 UVM gain (%)
1	PVC (flaming)	Ideal	5044569600	0.20	0.19	0.15	5.00	25.00
2	PVC (flaming)	Ideal	775733760	0.99	0.96	0.79	3.03	20.20
3	PVC (nonflaming)	Ideal	18129792000	0.09	0.09	0.06	0.00	33.33
4	PVC (nonflaming)	Ideal	2440174080	0.36	0.35	0.28	2.78	22.22
5	Wood	Ideal	983224320000	0.05	0.04	0.03	20.00	40.00
6	Wood	Ideal	280376064	2.83	2.79	2.10	1.41	25.80
7	PVC (flaming)	Albedo-only	3269176320	0.47	0.46	0.29	2.13	38.30
8	PVC (flaming)	Albedo-only	452676864	1.78	1.73	1.47	2.81	17.42
9	PVC (nonflaming)	Albedo-only	12816076800	0.51	0.50	0.20	1.96	60.78
10	PVC (nonflaming)	Albedo-only	1508636160	0.67	0.66	0.50	1.49	25.37
11	Wood	Albedo-only	3532984320(*)	1.82	-	-	-	-
12	Wood	Albedo-only	160250112	5.09	5.01	3.79	1.57	25.54
13	PVC (flaming)	Realistic	3491174400	0.29	0.29	0.27	0.00	6.90
14	PVC (flaming)	Realistic	463219200	1.71	1.65	1.58	3.51	7.60
15	PVC (nonflaming)	Realistic	11861606400	0.12	0.11	0.11	8.33	8.33
16	PVC (nonflaming)	Realistic	1609628160	0.56	0.54	0.52	3.57	7.14
17	Wood	Realistic	699475200000	0.06	0.06	0.04	0.00	33.33
18	Wood	Realistic	160167168	5.28	5.20	4.02	1.52	23.86

(*) 40 runs.

Fig. 6.6.: Bar plot showing per particle interaction simulation times for different setups. Setup numbers (#) correspond to those in Table 6.2.

The simulation times (normalized per particle interaction) corresponding to each condition are shown in Table 6.2 and represented in Figure 6.6 for clarity. The first conclusion is that CUDA6 versions are faster than the CUDA5.5 version. The CUDA6-MAN version, corresponding to the original CUDA5.5 code compiled using the CUDA6 Toolchain is slightly faster. This fact can be due to improvements in the compiler. Those differences mean improvements in the range of 2-5%, reaching 10% in some particular cases.

However, the most impressive gain comes when comparing the CUDA6-MAN version with the code using UVM (CUDA6-UVM in the table). In this case, gains in the vicinity of 25% are common, reaching 40% and in particular cases up to 60% (setups #5 and #9). However, big variability can be expected: they depend on the mean free path between wave-particle interactions. These in turn determine the mean number of operations per thread. Lower gains (about 5%) can be expected for lighter smokes and bigger mean free paths –fewer memory accesses–, while much higher gains (even above 50%) can be expected for denser smokes with lower mean free paths and higher amount of operations per thread –more memory accesses–. This fact can be easily explained by the fact that the longer runtimes of the CUDA kernel code, the more impact in the overall runtimes, as the relative impact of reading input files or writing output is minimized.

6.4.2. Targeted simulations

In order to gain some insight on the implications of the manual optimizations conducted, an additional series of tests were done. Kernel runtimes were measured considering:

- An atmosphere containing one, two or three particle types.
- The impact of the runtimes for one and ten runs of the model to gather information on the accumulated effect of the optimizations.

The results are depicted in Table 6.3 and show a recurrent issue when trying to optimize code: fitting code to a particular case may result in gains that may turn losses when applied to other situations.

In this case, manually optimized code outperforms UVM when only one type of particle is considered, but not otherwise. The reason behind this fact is that an increase in the number of particle types will result in bigger tables but a similar amount of memory accesses: in this context, gains can be expected for small tables as shared memory (L1 cache) is faster than L2 cache (tables in global memory are cached in L2 memory for the UVM case), both cases having low processor occupancy. On the contrary, more particle types mean more shared memory is needed and therefore occupancy is higher so less threads can run concurrently. In this particular case, only two blocks execute concurrently in the manually optimized version (in L1) for four blocks in the UVM case (in L2): the performance

Tab. 6.3.: Run times and manual optimization gains for targeted simulations.

Particle types	Number of runs	CUDA6-MAN (ms)	CUDA6-UVM (ms)	Time gain (%)
1	1	25.633	26.324	+ 2.70
2	1	27.840	26.496	- 4.83
3	1	34.882	26.990	-22.63
1	10	242.811	251.799	+ 3.70
2	10	259.745	242.038	- 6.82
3	10	330.342	251.672	-23.81

of the manually optimized version is severely affected.

In addition to the speed gains obtained for certain setups using UVM, it is important to remark the advantage of hiding data transfers to the average developer:

- Lower entrance barriers mean more people can access the computing power of a GPU with limited training.
- Code is easier to read and maintain, allowing shorter development cycles and rapid prototyping.

It is possible, however, to retain control of the data transfers between the GPU and the CPU, thus making it possible for advanced programmers and scientists to improve their codes using high-profile optimizations. In fact, another implementation taking the CUDA5.5 code as the basis was done in order to see if it was possible to match and beat the performance of the code using UVM. Using asynchronous memory transfers, optimizing occupancy in the GPU and playing with the amount of registers and shared memory per block it was possible to outperform UVM code. Those optimizations are nevertheless only valid for a particular hardware and a particular kernel or program: careful design decisions have to be made as it is a trade-off between speed and portability.

6.4.3. Lessons learnt: Performance enhancement and cost-effectiveness

In a highly competitive environment, the need for faster results may hide other non-technical factors that are crucial to maximize overall efficiency in real-world applications.

Optimization of the code is an iterative process which provides with less performance gains (in (%)) at a growing developing time in each iteration. For a real application, the developer and processor time and associated costs have to be taken into account. In fact, the optimization peak (this is, the optimum opti-

mization effort) may be expressed per unit time as follows:

$$\Delta t_{\text{devel}} \times C_{\text{devel}} = \Delta t_{\text{gained}} \times C_{\text{machine}} \quad (6.3)$$

where Δt_{devel} is the time necessary to improve the code, C_{devel} the developer cost, Δt_{gained} the performance gained and C_{machine} the cost of running the software, all per unit time. It is therefore wise to implement only cost-effective optimizations where the effort (left side of Eq. 6.3) is smaller than the benefit (right side).

The previous concepts, simple as they are, have important implications when applied to complex models or to cloud computing platforms, as a detailed evaluation of the costs incurred per unit simulation time is to be taken into account.

Last, it is interesting to enumerate the most important steps when finetuning a particular implementation:

1. Starting with UVM code is interesting as a first approach.
2. Gather knowledge of the time consumed by each part of the code: the NVIDIA profiler included with the nsight suite provides the developer with an excellent tool for such task. Setting suitable parameters and arguments which match real working conditions is very important at this point.
3. Gather knowledge of the hardware where the code will run, as well as its capabilities.
4. Optimize memory transfers by using asynchronous memory transfers, concurrent data streams and exploiting the memory hierarchy of the GPU.
5. Compute and optimize the CUDA occupancy taking into account maximum amount of registers to use, L1 cache vs. shared memory, etc. so that maximum throughput is achieved. Threads and blocks should not be resource-avid in order to allow more blocks to run concurrently in the same Streaming Multiprocessor (SM).
6. Look for the limiting factor, aided by the profiler but taking into account that the only one that really knows what is happening and what can/should be modified is the developer himself.
7. Run the profiler iteratively until a certain aim has been reached: the time devoted to optimization of the code must be coherent with the gain achieved.

6.5. Output and presentation

The potential amount of data generated by the model is very high and therefore it is important to choose which data is relevant and should be kept, and which other data can be safely discarded. With this idea in mind, three different output modes have been implemented:

- *Debug mode.* All the data generated is saved, current power, input and output directions of the photon bundle, as well as other metadata necessary for

Tab. 6.4.: Arriving tuples ordered by associated pixel.

Pixel number	Tuples: (power, time of flight)
0	$(\text{power}_0, t_0) (\text{power}_1, t_1) \dots (\text{power}_{n-1}, t_{n-1}) (\text{power}_n, t_n)$
1	$(\text{power}_0, t_0) (\text{power}_1, t_1) \dots (\text{power}_{o-1}, t_{o-1}) (\text{power}_o, t_o)$
$\vdots$	$\vdots$
n	$(\text{power}_0, t_0) (\text{power}_1, t_1) \dots (\text{power}_{p-1}, t_{p-1}) (\text{power}_p, t_p)$

the correctness of the model for every step of every thread. The amount of data generated in this mode grows very fast: this mode is used for debugging purposes and scarcely to get any useful information.

- *Array mode.* The “post-mortem” state registers (output direction, number of steps, power, distance traveled/time lapsed) for every pixel are saved. This includes data that do not contribute to the received signal, such as absorbed or transmitted bundles, as well as bundles that exit the simulation space.

This mode generates a rather big amount but highly valuable data. It gives insight into the space (or time) traveled by the photons before reaching the sensor or being absorbed/transmitted/etc. It also gives the number of iterations (number of times a particular bundle has reached a particle and interacted with it). Studying these figures it becomes possible to gain insight into the amount and importance of backscattering, smoke particle density, etc.

- *Aggregated mode.* In this mode, only the pixels activated from bundles that travel from the emitter to the receiver are computed. This way, only the “useful” bundles (those actually contributing with relevant information to the detected signal) are recorded. It does not provide basic information about the underlying physical processes but concentrates the data needed in order to visualize and make decisions about global parameters of the simulation.

6.5.1. Visualization of data

Taking the data gathered in aggregated mode as the basis, it is fairly straightforward to build images that give information about the raw data acquired by the sensor. To build such an image, the signals reaching the sensing element have to be ordered in a pixel by pixel basis. The result will be an ordered list of 2-tuples containing the time of arrival (time of flight) and the power of the arriving bundle for each pixel as shown in Table 6.4.

From there, it is relatively easy to extract further information on the signal: a

Fig. 6.7.: Per-pixel histogram showing times of flight vs. received power.

histogram is to be made where the respective bin width corresponds to the time resolution we want to have (see Figure 6.7). The value of the power for each time bin is obtained summing all the individual powers of the photon bundles received in that time interval. This way it is possible to simulate the effect of different time resolutions and also extract conclusions about the convenience of other post-processing techniques (such as gating), the dispersion in the sensing results as provided by different photon bundles, etc.

Once the histograms have been generated for each pixel, it is possible to present the information in an intuitive form by displaying it graphically: synchronizing the histograms for every pixel and assigning a relative intensity for a given power interval, 2D or 3D graphics can be created showing the result of the simulation in both qualitative and quantitative terms. Specially suitable for that task is the use of **the processing language** [268, 269], a programming environment aiming at promoting software literacy within the visual arts and visual literacy within technology.

As an example, a simple program has been implemented using processing. Taking simulation raw output files (in array or aggregated modes), a simple pre-processing step is performed: photon bundles not reaching the sensor plane are discarded as well as data not relevant for the visualization. In fact, only the following data is retained:

- *Traveled distance*: the space traveled by the bundle taking into account all the deviations incurred caused by scattering.
- *Number of steps*: the number of particle interactions undergone before reaching the sensor.
- *Power*: photon bundle power at the moment of detection.
- *Source pixel*: x - and y - coordinates of the originating pixel.

Fig. 6.8.: Screen capture of the visualization tool made in processing.

- *Destination pixel*: x – and y – coordinates of the pixel where the photon bundle is detected.

Once the data was sorted by traveled distance, two corresponding histograms were made and normalized: the first one showing the *aggregated power* of the photon bundles in a bin, and the second one corresponding to the *total number* of bundles received in the bin. In both histograms, the bins represent the amount of bundles that have traveled a distance in a certain time interval, which is depicted in the right frame for clarity as well. These histograms make it possible to relate the amount of pixels activated to their relative power weight for a certain traveled distance.

In order to gain more insight into the actual configuration of the received bundles at the sensor, a complementary graph showing the activated pixels at the sensor for the traveled distance interval (bin) active is drawn (upper left frame). In this graph, the pixels activated are colored depending on their relative power (more intensity corresponds to a more powerful detection).

A screen capture of the visualization tool showing the histograms and the sensor can be seen in Figure 6.8.

6.6. Concluding remarks

The model presented in the previous chapters has been implemented in a GPU for maximum performance. Due to the memory intensive nature of the algorithm, it is important to maximize memory throughput by optimizing memory use and transfers. In that sense, special care has been taken in the design of data structures. The nature of the algorithm itself, aided by the lack of interaction between threads, has made it possible to obtain reduced simulation times due to parallelization.

Two approaches have been discussed, one making use of manual optimizations and another one letting the compiler choose. Manual optimizations can yield better results for a narrow set of contour conditions. On the contrary, if the hardware or the specific features of the data are not precisely known, it is better to let the compiler decide, or else do the optimizations in two steps (automatic-manual).

A software graphical tool to analyze and visualize data has been presented as well. It is a convenient tool that allows the user to extract quality information from the simulation easily. It is an elegant solution that serves as a data reduction and a graphical decision tool. Despite being in its infancy, it can be a valuable aid in the early stages of the design of special-purpose gear serving as an artificial vision aid in harsh environments.

7. Model validation

"In theory there is no difference between theory and practice. In practice, there is."

Yogi Berra

Optical scattering has been one of the most extensively studied phenomena in Physics in the last two centuries. Extensive research on the topic is still going on, which means new instrumentation is needed to validate emerging computational models.

It is important to have experimental evidence supporting the validity of physical models, as this is the only way to prove their correctness and the accuracy of the results obtained. Every model implies abstraction and as such, simplification of reality through a finite set of variables that attempt to predict the behavior of a real system under certain circumstances (model scope). The design and realization of the experiments must give and take strategy, in order not to affect –or affect the least possible– the phenomena under study [270, 271].

The main objective of the experiments conducted within a validation framework is to assess the correlation between observations and simulations. The most convenient approach in this case is to design an experiment with elements that can be simulated well and the other way round: the experimental setup has to be designed to match the mathematical frame conditions as accurately as possible in a meet-in-the-middle approach.

In that sense, the easiest setup would involve the creation of a controllable and measurable medium. As we will see, in practice it means using sphere-shaped particles. A method to create synthetic calibrated dispersive media ("synthetic smoke") at a microscopic level using microspheres is developed to satisfy that need. A creative approach making use of additive manufacturing (3D printing) for rapid and ad-hoc prototyping of the components of the instrumentation, as well as for cost effectiveness is used and discussed below.

The following sections will dive into the details of the validation process itself, from the design and fabrication of the experimental setup to the discussion of the results. First, an overview of the validation setup will be given, along with the design of the experimental setup, subsystem by subsystem (optical, data acquisition, smoke chamber, etc.). Some optimizations actually implemented will

be discussed. Next, the fabrication process and the details of the parts involved will be described. Last, the data acquisition process and its comparison with the results predicted by the simulations will be analyzed. The detailed description of the steps needed for the generation of the scattering atmosphere can be found in Annex C.

7.1. Related work

Two of the most relevant approaches to the measurement of scattering found in the literature take an opposite direction: on the one hand the measurement of macroscopic optical constants (see for example [272]), and on the other hand the measurement of the scattering properties of individual particles (see [273] for a review on the subject). A simple search will provide the interested reader with many relevant references in different scientific domains. In addition, the need for a controllable and reproducible medium assimilable to smoke to make the measurements has been appreciated before. Expert panels have discussed the possibilities of having soot reference materials for instrument calibration [274]. The custom fabrication of optical parts for experimentation has been addressed before as well [275], in line with a growing trend in low-cost scientific [276] and Do It Yourself (DIY) electronics [277]. However, there is no evidence to date of precision experiments conducted using those components.

In this chapter, the custom design and fabrication from scratch of an advanced instrument is presented following a multidisciplinary and multiangle approach. It has been designed with advanced techniques such as parametric design [278] and fabricated with additive technologies [279]. The simple but versatile method to create calibrated synthetic smoke (at the microscopic level) has not been found elsewhere in the terms proposed in this thesis and can be of use in manifold applications. These ideas will be discussed in detail below.

7.2. Validation scope, limitations and system overview

The full validation of the system would require the quantitative and qualitative measurement of the optical power received at the sensor –including the position and intensity of the pixels actually activated–, along with timing data (see Figure 7.1).

Although the capabilities of the model go further beyond, a simpler experimental setup is proposed (shown in Figure 7.2). A single-pixel emitter with the corresponding optics and electronics will be used to obtain a small profile beam

Fig. 7.1.: Concept setup for the experiment and data provided by the model.

Fig. 7.2.: Conceptual setup showing the physical blocks needed: 1. Optical bench and supports; 2. Emitter and driver electronics; 3. Optical hardware; 4. Confined space for the medium; 5. Medium injector; 6. Air filter; 7. Sensor and data acquisition.

for injection into the medium chamber. The chamber is where the interaction between the incident radiation and the scatterers takes place. The sensor, placed at the far end of the chamber and facing the emitter, will read the intensity of the signal received in each of its pixels and process it. A particle injection system, which includes an air filter is necessary as well. This is a simple way to measure the intensity and position of the signal received and answer two of the basic questions addressed by the model regarding the signal received (see chapter 5): “*where?*” and “*how much?*”.

The question regarding timing, “*when?*”, would need a different setup and very fast electronics to deal with delay times in the subnanosecond range—light round-trip times for paths in the meter range— if time of flight is to be measured directly. Different emitters and sensors would be needed to handle these propagation and arrival times properly.

The emitter would have to generate light pulses, either using pulsed sources or a specific chopper. The sensor could consist of an array of photodiodes connected to a device fast enough to be able to record the differences in propagation times

Fig. 7.3.: Alternative setup for TOF validation: 1. Single-pixel emitter (LED); 2. Smoke chamber (medium); 3. Optical receivers (lenses); 4. Optical fibers with different lengths for different delays τ_1, τ_2, τ_3 ; 5. Photodiodes; 6. ADCs with high-speed sample-and-hold and DSP; 7. Data processing.

accurately in the subnanosecond range. Those intervals cannot be measured using conventional Complementary Metal–Oxide–Semiconductor (CMOS) sensors due to normal response times (the analog output for each pixel is needed in order to measure differences in arrival times). Further data processing (i.e. the use of cross-correlations and indirect time-of-flight measurements) could leverage these requirements, but still high precision hardware is needed to ensure reproducible and sharp slopes in pulsed sources, etc [280].

An alternative setup able to measure and validate timing data provided by the model is depicted in Figure 7.3. In it, a single-pixel emitter (single Light-Emitting Diode (LED)) [1] injects optical power into the medium chamber [2]. Opposite the emitter, a battery of optical receivers detect the incoming radiation [3], once scattered by the medium. They can be connected to optical fibers of different, known lengths [4] that are in turn connected to photodiodes [5]. A battery of sample-and-hold Analog-to-Digital Converters (ADCs) [6] can benefit from the calibrated delays introduced by the optical fibers in order to extract the differences in arrival times between receivers after data processing such as autocorrelation [7]. This setup would still require high speed electronics with stable delays (high-quality ADCs, high-speed samplers, etc.). Timing is left out of the validation scope at this stage.

The experimental setup makes use of ad-hoc designed components combined with high-end consumer-grade and professional hardware. This way, it is possible to obtain relevant data while keeping fabrication and experiments quick and cost-effective. This bottom-up integration has clear advantages: it will be possible to define and control every step of the process. It also has disadvantages, mainly derived from the use of non application-specific hardware: there will be limits in terms of resolution, as the dynamic range and the limitations of the lenses and acquisition gear yield less precise results than the numerical values offered by the model.

Given the framework nature of the model –which makes it possible to simulate arbitrary particle concentrations and size distributions–, it is necessary to choose a set of representative cases of study. It is not feasible to validate every condition

that can be met due to the number of variables necessary to define each setup. In addition, the dynamic nature of smoke and the tendency of smoke particles to aggregate makes it necessary to produce a number of smoke setups that can be both reproducible and stable during the tests. Hence the need of synthetic smokes (i.e. scattering atmospheres) made of particles with known optical properties. This does not affect the generality of the model: any type of smoke can be simulated, as long as its properties are well-defined (total concentration, types of particles, their relative concentrations and the optical properties of the individual particles). The model will need that information as well as other parameters such as temperature of the medium, wavelength of the incoming radiation, etc.

As said before, the emitter will be restricted to one pixel. This goes without loss of generality either: it allows higher control of the incident radiation and possible sources of error that could interfere with the final result and may not be attributable to the model itself. The emitter will be placed in one end of the simulation chamber and the sensor in the other. No intermediate objects have been incorporated in the setup at this point to avoid sources of error.

Last, the model considers an ideal ray of light, propagating along a direction and without a cross-sectional distribution of power. A real beam may introduce errors when comparing the results obtained in the experimental setup with the simulated ones.

7.3. Instrumentation design

The proposed experimental setup consists of a series of elements aligned so that the optical radiation goes from the emitter to the sensor. Those elements are listed below and are basically coincident with the conceptual setup in Figure 7.2. Their design and particularities will be discussed in the following sections:

1. Optical bench and supports.
2. Emitter and driver electronics.
3. Optical hardware.
4. Confined space for the medium.
5. Medium injector.
6. Air filter to prevent the particles from leaving the medium chamber.
7. Sensor and data acquisition.
8. Data gathering and processing.

It is also important to pay attention to the design of the joints between the different parts of the system: their performance will impact notably in the reliability of the results obtained.

7.3.1. Optical bench and supports

There are a number of specialized firms that provide professional optical benches. The same holds for supports, taking into account that each firm designs supports in general only fully compatible with their own gear.

In our case, an optical bench was designed and fabricated ad-hoc for the experiment in a search for a custom and tight budget solution.

A steel-made 1500mm European standard IPN100 beam was prepared and cut to the task to serve as frame for the optical bench. The maximum tolerable straightness deviance for an IPN100 to comply with the BS EN 10024:1995 norm is $0.3\%L$, where L is the length of the original beam. The observed value was much smaller than the 4.5mm permitted by the norm. Its weight is 8.32kg/m, for a total 12.48kg. The bench was completed with a 35mm stainless steel right angle bar welded on top of the beam forming a sort of “roof” (with tolerance $\pm 0.4\text{mm}$). The angle weighs 2.17kg/m, for a total 3.26kg. The optical bench’s total weight is therefore 15.74kg, heavy enough to ensure stability. A meter with millimeter divisions was added as well to be able to reproduce the position of the holders across different experiments. Neoprene damping sheets were also included to minimize the effect of vibration on the measurements. The design, inspired in commercial counterparts, is depicted in Figure 7.4.

The supporting gear for the lenses and electronics was designed and modeled in collaboration with the 3D specialist *archiologics studio* [281] using the state-of-the-art software package RhinocerosTM v.5.0 [282] to model the different parts. The aim was to have interoperable and reliable, yet simple parts that could be adjusted in height and kept in a fixed position easily while making measurements.

The supports were designed in blocks, so that few designs could be combined to build many different supports following a “design expandability” philosophy, similar to LEGOTM [283] building blocks. The parts were custom designed using parametric design techniques to fit the optical bench above. To avoid assembly errors, the bases were asymmetrical by design.

The supports consist of a set of four parts (base, base cylinder, inner cylinder and holders of several types) as seen in Figure 7.5.

- *Base*. It serves as support by matching the shape of the optical bench. It has two holes in its bottom to host two 4.8-5.5mm screws that fix the support against the optical bench, preventing it from moving along. In its upper part it has two male squared connectors to receive the base cylinder or corresponding part.
- *Base cylinder*. It consists of an empty cylinder that can be filled with another smaller cylinder. In its upper part it has a hole to host a 4.8-5.5mm screw to adjust the height of the inner cylinder.
- *Inner cylinder*. It is a smaller cylinder that works as a telescopic arm. In

(a) Scheme.

(b) Photo: bench with supports.

Fig. 7.4.: Custom optical bench designed and built for the experiments.

Fig. 7.5.: Support system and assembly process. Base (right); Base cylinder, inner cylinder and holder (left).

its upper part it has a squared male connector (the same connector system as for the base) to receive further accessories. A pass-through hole near its head makes it possible to use plastic ties to secure the pipes or other gear to the supports.

- *Holders.* Different types of holders were designed for the particle chamber, optics and other gear: 50mm and 25mm pipe holder, flat holders, etc. They all have a female square connector at its bottom to ensure perfect connectivity with the inner cylinder.

Annex A contains 3D plots of the different parts designed in the experiments along with their dimensions.

7.3.2. Emitter: optical source and optics

The generation of a suitable optical signal is critical to ensure high quality, reproducibility and correlation of the experiments with the model. The ideal light source would combine high power density with good spatial coherence and no artifacts such as speckle. The first source of choice is therefore high power LEDs, as –unlike lasers– they do not suffer from speckle noise. Besides, they emit narrowband light and are available for a wide range of wavelengths at affordable prices. Promising advances in random lasers will allow speckle-free full-field imaging in intense optical scattering [284], ideal for these experimental setups.

Fig. 7.6.: 3D printed holders.

Tab. 7.1.: Properties of the LEDs chosen for the experimental setup.

	Red	Green	Blue
Manufacturer	Osram	Osram	Osram
Model	LR CP7P-JSJU-1	LT CP7P-KXKZ-25	LB CP7P-GYHY-35
Wavelength (nm)	623	543	476
Output power (lm)	56.3-71	45-112	21-39
Forward current (mA)	100-1000	100-1000	20-1000
Forward voltage (V)	2.0-2.6	2.7-3.7	2.75-3.5
Beam width (°)	80	80	80

A list with the properties of the LEDs considered is shown in Table 7.1. Power LEDs emitting at three different colors (red, green, blue) were finally chosen from an initial group of five: the IR and the UV LEDs tested were small-signal LEDs, being discarded for not having enough power for the experiment. The ones chosen exhibit high output power at the cost of lower directivity $\sim 80^\circ$ compared to 15° of the small-signal LEDs. This fact has an impact in the design of the optics necessary to drive an adequate amount of optical power into the particle chamber in the form of a very narrow beam. Given the ideal character of the incident ray of light in the model, a high power LED is necessary to ensure enough power density at the sensor.

The LEDs used as light sources determine the forward current and voltage needed to drive them. Driver circuits were also designed in order to obtain the maximum output power. Figure 7.7 shows the relative spectral emission for the LEDs used with $\Phi_{\text{rel}} = f(\lambda)$; $T_s = 25^\circ\text{C}$; $I_F = 350\text{mA}$. Data taken from [13].

Due to the importance of generating and maintaining a stable atmosphere in

Fig. 7.7.: Relative spectral emission for the LEDs used in the validation setup. Taken from the manufacturer's datasheets [13].

the particle chamber, the measurements should be made as fast as possible. In order to compare the results of the scattering obtained for each of the incident radiation wavelengths for a given atmosphere, an additional idea was implemented to minimize the time taken for a series of experiments sharing a single particle configuration and three wavelengths. See section 7.3.7 for a detailed explanation. A system able to flash the three source LEDs consecutively is required.

The use of power LEDs needs specific (i.e. more powerful) current drivers. These were designed to be controllable by an Arduino[®] UNO and capable of driving the currents required. The circuits make use of an LM317, a well-known voltage regulator able to drive currents up to 1.5A (see Figure 7.8). The LM317 fixes 1.25V between V_o and V_{adj} , which makes it easy to drive a LED, as I_{adj} is almost negligible:

$$I_o = \frac{V_o - V_{adj}}{R3} = \frac{1.25V}{R3} \leadsto R3 = \frac{1.25V}{I_o(A)} \Omega \quad (7.1)$$

$R3$ will depend on the I_o of choice. For instance, for $I_o = 0.5A$, $R3 = 2.5\Omega$. Setting $V'_{in} > 3V$ (the recommended values for $V'_{in} - V_o$ are between 3 and 40V) forces $V_o - V_{adj} = 1.25V$, where the recommended values for V_o are between 1.25 and 7V. Therefore, the forward voltage of the LED used will determine V'_{in} .

In addition, it is possible to modify this circuit to drive the three LEDs using

Fig. 7.8.: Basic high current, Arduino-controllable LED driver.

Fig. 7.9.: Full Arduino-controllable high power RGB-LED driver.

a single LM317 shared among them and adding simple electronics to switch on or off the particular branch by setting the proper value at the Arduino's GPIO pin. Figure 7.9 shows the final circuit. R_a fixes the current that will be supplied to the LEDs according to the calculations above. R_{in} is the internal resistance of the voltage source V_{cc} . R_2 , R_5 and R_7 condition I_c and therefore I_D in each branch. $R_1 = R_4 = R_6 = 4k7\Omega$, which is an appropriate value for the interface with the Arduino GPIO ports (GPIO11, GPIO12 and GPIO13 for D1, D2 and D3). The transistors should have collector currents high enough to be compatible with the LED. For convenience, $Q_1 = Q_2$, $Q_3 = Q_4$ and $Q_5 = Q_6$. All six transistors can be equal. It is important to grant that at any given time no more than one branch is active or otherwise the LM317 would not be able to supply enough current. This was accomplished leaving all branches off for 2ms (between changes). Each LED was consecutively on for 300ms, so only one LED was on at a given time. The Arduino code is available upon request.

Once the radiation sources can be controlled, it is time to conform the radiation pattern to obtain a light beam that matches the model as close as possible: a

collimated and small profile, narrowband beam must be obtained. As said, the LEDs used for the experimental setup had relative high output power (75mW) with wide beams (80°). Thus, the first task to tackle is to adapt the radiation conditions of the LED to match the model as much as possible. This process involves two steps: collimating the beam and spatially profiling it (see Figure 7.10):

- **Collimation:** An adequate focal length and lens diameter must be used, taking into account the physical dimensions of the LED and its radiation diagram. The focal length is given by equation 7.2, where α is the angular aperture of the radiation source.

$$f = d_{\text{beam}} / (2 \tan(\alpha/2)) \quad (7.2)$$

The idea is to use a Plano ConveX lens (PCX) able to collect the light emitted from the LED within a wide solid angle, thus achieving a beam of collimated light with high power density. A diameter of 20mm was chosen for the PCX lens as a good trade-off taking into account manufacturing reasons. The focal length of the lens must be chosen considering the radiation pattern of the LEDs used in the experiment. Finally, an Edmund Optics 45499, PCX with D=20mm, f=20mm, NA=0.5 was chosen.

That value is convenient in terms of manufacturing and beam collimation: the diameter of the PCX lens has been selected to obtain the highest power density possible after the spatial profiler, considering the LED beam width, the diameter of the pinhole and the focal length. It is important to consider as well that the projected beam of the power LEDs on the PCX lens exceeds the surface of the lens itself. This is due to the radiation pattern of the power LEDs (80° width): a certain amount of *stray light will be added to the experiment*. Divergence was also considered: real world calibration results (measurements without scattering atmosphere) gave low divergence patterns.

- **Spatial profiling.** A pinhole aperture can serve as a good spatial profiler, adding spatial resolution to the incoming collimated beam. This comes, however at a cost: again, the power emanating from the pinhole will be much lower than the incoming one, as a significant part of the incoming radiation will be absorbed or reflected at the aperture walls. An Edmund Optics 56276, 10 μ m aperture diameter, mounted, precision pinhole was used for the experiment, a size comparable to one pixel in many CMOS cameras. Considering this diameter ($d_{\text{pinhole}} = 10\mu\text{m}$) and an incoming beam diameter $d_{\text{beam}} = 20\text{mm}$, the resulting surface ratio (S_R) –equivalent to the *power ratio*–, would be 2.5E-07:

$$S_R = \frac{d_{\text{beam}}^2}{d_{\text{pinhole}}^2} = \frac{P_{\text{LED}}}{P_{\text{out}}} \quad (7.3)$$

Equation 7.3 stresses the importance of a powerful radiation source: the

Fig. 7.10.: Ideal optical processing scheme of the emitted radiation to obtain a collimated and spatial profiled beam.

power effectively radiated into the particle chamber gets reduced by seven orders of magnitude, the exact final power depending on the features of the device used. This is the reason why only high power LEDs were finally used for the experiment.

The optics and the electronics were assembled together into a compact holder to be attached to the particle chamber, resulting in a system capable of generating a micron range-wide light beam from a high power LED.

Optical and electronics subsystems were put together using high pressure PVC pipes and parts, as they are widely available, cheap and provide a perfect fit for the pinhole aperture and the lens. The overall scheme is shown in Figure 7.11: light emanates from the LED positioned in #4 and goes all the way down to #18 through the lens and the pinhole.

Finally, the electro-optical subsystem must be coupled to the particle chamber with a means to prevent the injected particles in the chamber from leaving while allowing the optical radiation in. Covers were custom designed using 3D modelling. They will be explained in more detail in the following sections.

7.3.3. Simulation chamber

The model has a configurable virtual environment in which the simulations take place. The reason for this is the need for boundaries: photon bundles traveling away from the emitter-sensor line of sight must be extinguished somehow. It is necessary to consider that backscattering can be relevant under certain conditions; the photon bundle may be redirected back to the line of sight emitter-sensor and therefore a simulation space big enough but of reasonable size is needed (a space between one and two orders of magnitude bigger than the sensor is enough for our purposes).

In the real setup, it would be certainly easy to build a container many orders of magnitude bigger than the sensor. However, due to the high price of calibrated microspheres for use as scatterers (see section 7.5), it is necessary to use smaller

Fig. 7.11.: Optical radiation subsystem (section): 1. LED connectors; 2. LED PCB holder; 3. LED PCB; 4. Active LED aligned (other LEDs marked in grey); 5. Eccentric part; 6. 20mm PCX lens; 7. 20mm PVC socket; 8. 10µm pinhole; 9. 25mm PVC socket; 10. 25/20mm PVC reducer; 11. 20mm PVC pipe; 12. 20mm PVC socket; 13. Microfilter and chamber interface; 14. 50mm PVC pipe; 15. EVA sponge seal; 16. 50mm cover for microfilter; 17. EVA sponge seal; 18. Particle chamber.

Fig. 7.12.: Setup proposed for validation.

recipients (such as pipes) to make the experiments affordable. In any case, the simulation chambers used in the experimental setup were at least one order of magnitude bigger than the sensor.

The experimental setup used for validation is shown in Figure 7.12. It has been simplified to avoid as many error sources as possible. For instance, there will be no objects in the simulation chamber. In addition, the emitter will face the sensor: this way the experiment will be focused on assessing the performance of the model in terms of the optical characterization of the smoke or particle-filled atmosphere. The simulation environment has been adapted accordingly to mimic the experimental setup.

High pressure PVC pipes were used for the simulation chamber. A number of reasons supported the decision:

- They are a good trade-off between internal volume, size and versatility at a reduced cost. This way the scattering path can be easily varied using pipes with different lengths.
- They are cheap and easy to mechanize (cut, make openings, etc.).
- They are round and so they have no corners (except for the endings). This prevents microspheres from being trapped and favors the flow of the scattering medium when being introduced in the chamber.
- They are black or dark, resulting in reduced reflections of the incoming radiation at their inner surfaces.

The use of PVC high pressure pipes with diameter sizes of 25 and 50mm is convenient, as they provide with enough simulation space (more than one order of magnitude bigger than the sensing device and much bigger than the incident beam width) while retaining good maneuverability and a relative low number of microspheres per test for a given mean free path.

Fig. 7.13.: (a) PARI Nebulizer and compressor. (b) Nebulizers for different droplet sizes: $2\mu\text{m}$ (red - left), $3\mu\text{m}$ (yellow - center) and $7\mu\text{m}$ (uncolored - right)

7.3.4. Particle injection and air flux

The particles injected in the chamber must be confined to avoid possible leaks. Besides, after the injection of the particles, the atmosphere in the simulation chamber must remain as stable as possible. Therefore, it is necessary to design a system that grants a constant air flux while these particles are injected, and a means of injecting the particles inside the simulation chamber so that they cannot leave the confined space.

Particles will travel nebulized inside droplets of similar size acting as their “volatile vehicles”. It would be desirable to generate aerosols with calibrated droplet sizes close to particle sizes. The idea is to leave an atmosphere as stable as possible once the appropriate amount, size distribution and type of particles has been injected into the chamber.

The method to inject the particles comprises a series of steps:

1. Design and calculation of the number and types of particles to inject into the chamber. The procedure is written in detail in Annex C.
2. Preparation of the solution of the particles in an appropriate carrier in order to feed the nebulizer with the concentration and volume required by the manufacturer.
3. Injection of the particles using the nebulized solution, and wait for the carrier to evaporate.
4. During the previous step, the atmosphere should have become stable. If not, it is necessary to wait for it to settle (see Annex C.2 for reference times).
5. Run the experiments.

The problem of launching the scatterers into the pipes is that of suspending in air particles in the micron range. Nebulizers used in medical applications are

Fig. 7.14.: Air and light flux directions inside the particle chamber (air flux shown with thinner arrows, light flux with one thick arrow): 1. Air inlet; 2. Excess air outlet (with microfilter); 3. Light inlet; 4. Light sensor.

very effective at suspending particles in the range of $3\text{--}5\mu\text{m}$ ¹. The principle of operation of some of those nebulizers is as simple as a specially crafted venturi that makes particles leave a recipient with the drug solution and collide with a plastic part designed to produce particles in that size range. The antibiotics would then travel inside a droplet of solvent of the proper size to reach the alveoli.

It is not easy to find nebulizers that generate calibrated droplets of the size required for the experiment at relative low pressures and air velocities. One model that does is the PARI LC nebulizer [285], which consists in an air compressor plus a set of PARI LC Sprint reusable nebulizers for different mean particle sizes: 2, 3 and $7\mu\text{m}$ (represented in Figure 7.13).

The injection of the aerosol into the simulation chamber needs to be carefully supervised to prevent overpressure. Not only the pressure inside the chamber must be kept low, but the aerosol flux should be as laminar and regular as possible to create a uniform atmosphere to ease calculations and ulterior atmosphere stability. The seals and joints like #15 and #17 in Figure 7.11 make the chamber “particle-tight” and provide a way to evacuate air without causing turbulence, overpressure or other adverse effects (number #13): the excess air exits the chamber while the particles stay.

47mm MILLIPORE $0.22\mu\text{m}$ membrane filters (GSWP 047 00) were used to retain the particles while letting the air out. Light was decided to travel in the opposite direction to the air flux to ease manufacturing, measurements, and air flux itself (see Figure 7.14). The active surface of the filter had to be maximized while ensuring that the optical emitter and receiver were not affected. The design of the particle filter is explained in more detail in the next section.

7.3.5. Particle chamber endings and connections

As said before, the pipe serving as the particle chamber needs endings configured to let the light in while retaining the injected particles within the chamber. Figure 7.15 shows a scheme of the light inlet (corresponding to #1 and #4 in Figure 7.14) and excess air outlet (corresponding to #2 and #3 in Figure 7.14) as seen

¹They are the optimal sizes needed for antibiotics to reach the lower respiratory tract.

Fig. 7.15.: Pipe endings. Scheme for filter active surface and optical performance optimization.

from the particle chamber.

The light inlet corresponds to part #13 in Figure 7.11. It actually consists in two washers with the shape shown in Figure 7.15(b) with a microfilter membrane placed between them and properly sealed. A microhole is opened so that light can pass through the system unaffected. An additional EVA sponge washer is added between the pipe and the endings for enhanced sealing (see #17 in Figure 7.11). See Annex A for the technical drawings.

7.3.6. Acquisition hardware, configuration and procedure

Data acquisition is an essential part of any experiment and very specially here, as the precision of the data gathered has direct influence on the assessment of the validity of the model. In the experimental setup the sensor needed is a profile sensor or a digital camera, with as low acquisition times as possible, reduced sensor area, good pixel sensitivity and lenses (if they cannot be removed) that do not alter the received signal significantly.

High-performance profile sensors available in the market for light spot detec-

tion (such as [286]) combine high frame rates with 2D digital outputs at 8-10 bit precision, depending on the maximum frame rate. They are suitable for the task, but need dedicated support circuitry to run the circuit and nonuniform spectral response. Budget and timing restrictions forced the search for other options. Charge-Coupled Device (CCD) professional solutions or complete beam detectors were also examined but discarded for their relative low frame rate and bulky form factor.

A search was made looking for alternative options combining high frame rate with a suitable form factor at a reasonable precision and cost. Several models were tested and finally a high-end mobile camera was chosen: iPhone 6 working in burst mode at 10fps and in slow-motion mode at 240fps.

Fabricated by Sony, the iSight camera chip inside the phone is a stacked (Exmor RS), back-illuminated CMOS Image Sensor (CIS) featuring 1.5 μ m generation pixels. At 240fps, it takes about 4ms to take a picture. Although far from the frame rate of profile sensors (3200fps, about 0.3ms per frame) the quasi-static approach can still hold with limitations for the validation setup.

Further tests were made to assess the performance of the camera in the experimental setup, regarding noise and dark current. As a result, the maximum length of the smoke chamber was decided to be 40cm to ensure enough optical power was received at the camera sensor.

The location and attachment system of the camera for the experiments was also an important issue. Figure 7.16 shows the pipe ending (which corresponds to the scheme in Figure 7.15(a)) with its camera holder. It is very important to adjust the camera opening in the pipe ending to the camera lens to avoid particle leaks at this point. Additional seals –i.e. Ethylene Vinyl Acetate (EVA) sponge or plastiline– can be necessary. In any case, the camera needs to be fixed in its position using sargents or by any other means. The attachment of the nebulizer has also been considered in the design phase, ensuring maximum transfer of the generated aerosol to the simulation chamber.

The data obtained with this method (mainly still images) can then undergo further postprocessing to enhance their analysis and interexperiment comparison. This experimental setup can obtain qualitative results. Quantitative ones can be expected as well when different experiments are compared.

7.3.7. Optimizations and other additional considerations

A creative way of injecting optical power into the simulation chamber can help minimize the cost associated with every experiment if the same medium is illuminated with the three power sources (red, green, blue) consecutively. In addition, this procedure ensures a homogeneous scattering atmosphere through the tests: the smoke is stable for much longer than needed for the measurements (An-

Fig. 7.16.: Pipe ending with camera holder. The opening for the camera corresponds to the conic aperture.

Fig. 7.17.: PCB with the SMT LEDs and the eccentric part showing the position marks for each wavelength.

nex C.2 contains reference information on settling times). The implementation of the previous idea needs special-purpose parts and some electronics –as explained below–.

On the one hand, the LEDs were soldered to a custom circular PCB with all the connectors on its backside so that no part would interfere with the light emanating from the LEDs (see Figure 7.17(a)). A control unit would turn the different LEDs on and off ensuring only one LED was on at a time. This was implemented in practice with custom drivers designed for the LEDs chosen and an Arduino board acting as the controller (see section 7.3.2 for more details).

On the other hand, it is necessary to couple the electronics and the PCB to the system optics. The main idea is to align only one LED with the optics at a time, so that only the light emanating from that LED would make it into the smoke chamber. This problem was solved designing an eccentric part that would expose only one LED to the optics while blocking the other two. The fabricated part is shown in Figure 7.17(b). Please refer to Annex A for the technical drawings.

This “selective light routing” is accomplished in practice rotating the PCB holder manually so that the mark in the eccentric part is made coincident with one of the marks in the PCB holder. At that point, the corresponding LED is positioned matching the PCX lens and the pinhole axis, while the other two LEDs are kept away from the axis with their light partially blocked and out of focus.

The system provides a simple way of maximizing experiment throughput and comparability while minimizing particle configuration errors from experiment to experiment.

7.4. Fabrication of the parts

The experimental setup as a whole has been conceived with fabrication in mind in all design phases. Thanks to novel 3D modelling techniques, and specially parametric design [278], it was possible to adjust tolerances in the 3D printing process easily to obtain high quality parts in days. Parametric design makes use of scripting and parameterization to automate construction, industrial designs, generate structures, etc. The 3D modelling of the parts was done with Rhinoceros5.0 [282] and Grasshopper [287].

A set of calibration parts was also designed and manufactured to measure the actual tolerances of the fabrication process. This way it was possible to feed the parametric model to optimize plastic use, energy and 3D printing time for rapid prototyping. The fabrication flow comprised the following steps:

1. Paper and pencil design.
2. Modelling of the parts identifying the most relevant parameters susceptible of adjustment during the prototyping phase.
3. Creation of the parametric and 3D model of the part.
4. Optimization of the placement for fabrication, considering that beyond a certain angle –up to 62° has proven to work– the 3D printer cannot “print in the air” and thus needs supports that must be removed after fabrication. It is important to set the properties of the supports carefully so that they can be removed easily and that not much postprocessing is necessary: hard to remove supports need more work and have influence in the final quality of the part, in some cases making it unsuitable for the task. This is another variable to take into account during the design process.
5. Processing the 3D models into 3D printing instructions. The printers used were GCode-based. Software such as CuraEngine [288] and Repetier [289] were used for this task. Parameters like printer type and nozzle diameter (tolerance adjustments) had to be optimally configured as well.
6. Print the part. The use of calibration parts and parametric design techniques saved a considerable amount of time, as it allows to double check tolerances between different printed parts.
7. Removal of the supports where applicable.

7.4.1. 3D printing

Several materials and printers were used during the design and early tests phase. Finally, a Makerbot II 3D printer with 1.75mm PolyLactic Acid (PLA) as the printing material was chosen. A layer height of 0.15mm was used for maximum quality. CuraEngine configurations are available upon request.

In addition to the placement of the individual parts for support minimization, it is important to pay attention to the layout in the printing bed when combining several parts to be printed at once. Not only the 2D placement, but the 3D shape of the parts must be taken into account. The aim is to minimize the number and length of extruder travels: a slight improvement in placement results in significant printing time reductions. At this point there is software for automatic nesting of 2D parts for laser cutting or Computer Numerical Control (CNC), but –at the time of writing–, none yet for 3D printing. The placements must therefore be optimized manually.

7.4.2. PVC pipes and parts

The use of high pressure PVC pipes makes it possible to develop prototypes quickly and easily. Besides, the availability of sockets and pipes of different sizes (20, 25 and 50mm) makes it possible to build systems with matching pieces easy to assemble. Moreover, PVC makes it possible to cut or adapt pipes and parts to the setup easily.

The use of transparent pipes during the design and early test phases made it possible to observe the influence of particle injection inlet positions in the quality of the final atmosphere generated and measure the time intervals for nebulization, settling time, etc. to be used with opaque PVC pipes in the real experiments. This had also positive implications in the design of the experimental setup and the overall quality of the experiments.

7.4.3. PCB board and electronics prototyping

The electronics were simulated using the PSPICE models for the circuit in Figure 7.9. The General-Purpose Input/Output (GPIO) inputs correspond to the digital outputs of the Arduino UNO board. As stated in section 7.3, the power LEDs were placed in a circular PCB board designed to fit the cover of the eccentric part. The PCB was designed with Altium Designer [290] and later sent for fabrication using standard practices. Care was taken to ensure that the PCB with the SMT LEDs could turn 360°, ensuring this way each LED could reach a position coincident with the lens axis. See Figure 7.17.

As stated above, the combination of the electronics controlled by the Arduino board and the positions of the LEDs –manually set turning the eccentric cover– made it possible to perform the measurements corresponding to the three wavelengths studied (red, green, blue) with the same atmosphere in the particle chamber. This has positive implications already explained.

7.4.4. System calibration

The tolerances of the fabrication process are well controlled and below 0.15mm after the adjustments made in the prototyping phase. Therefore, the errors due to fabrication mismatches are small enough to consider only minor calibration. When it comes to the scattering measurements, simply adjusting the beam at the center of the image taken by the camera before injecting the particles in the chamber was enough. This calibration served as a later reference when particles had been injected and the image received was altered.

7.5. The medium: design, synthesis and injection

It is important to recall that our model needs the scattering profiles of the particles in the medium, irrespectively of the type of particle or how that profile was obtained. Furthermore, a reference medium serving as a pattern is necessary in order to validate the model.

The obtention of a smoke-like atmosphere with known and reproducible optical properties is essential to the validation process and no trivial task. After a thorough analysis of several possibilities such as the generation of real smokes from controlled fuels, it was decided to create a synthetic smoke made of artificial particles with known and precise optical and geometrical characteristics.

Given that the scattering profiles of particles can be predicted only for certain geometries, it seems wise to use homogeneous spherical scatterers: their scattering profiles can be easily calculated using Mie theory. They have an additional advantage over other geometries or, in the most common case, fractal shapes: they “look” the same in terms of optical properties irrespectively of the angle of incidence of the incoming radiation. This is convenient, as there is no need to consider the scattering diagram for every possible position of the nonspherical particle.

The generality of the model is not affected at this point, as what is needed is a real environment that can be as reproducible and close to the simulation environment as possible: the aim is to detect discrepancies between the values obtained in the simulations and those measured in the experiment.

There are several manufacturers that offer monodisperse microspheres for research purposes which meet our requirements. They are available in different sizes and materials, and are widely used in the biochemist research industry. For the experiments, polystyrene microspheres from Ikerlat Polymers [291], Sigma-Aldrich [292] and Polysciences [293] were used. Please refer to Annex C for more details on the design and implementation of the scattering medium.

Monodisperse microspheres are injected into the simulation chamber using a

Tab. 7.2.: Volume of commercial solution needed for each setup.

Particle size diameter (μm)	Volume (μl) MFP = 200mm	Volume (μl) MFP = 100mm	Volume (μl) MFP = 50mm	Nebulizer type (μm)	Final volume in nebulizer (μl)
1	12.56	25.12	50.24	3	500
2	97.56	195.13	390.25	3	500
3	155.19	310.39	620.78	4	1000
6	354.52	709.04	1418.07	7	2000
Mix	0.14/46.03/153.44	0.28/92.06/306.88	0.57/184.13/613.76	7	1000

volatile carrier (methanol) and the medical nebulizer described in Section 7.3.4. It is necessary to wait for a period of time (t_{evap}) before proceeding with the measurements –see Annex C.2–.

Given the tiny amount of microspheres needed for some setups (those with longer mean free paths), it is necessary to add some more pure methanol into the nebulizer to ensure proper operation (see Table 7.2). In addition, nebulization times have to be recomputed for the final amounts of suspension in the nebulizers.

The evaporation time (t_{evap}) is also adjusted, as the amount of carrier to evaporate (methanol) will be smaller when the microspheres are injected in the chamber –the volume of methanol will correspond to the volume occupied by a spherical crown with thickness $r_{\text{aerosol}} - r_{\text{microsphere}}$ (r_{aerosol} is the radius of the particles in the aerosol)–. In this case, a conservative value for t_{evap} is 30s.

It is important to remark that once evaporated and given its low reactivity, methanol is a molecule whose cross-section is in the vicinity of 300pm: it has therefore a negligible influence in the measurements.

7.6. Data obtention procedure

The first thing to calculate is the precise amount of commercial suspension needed for each experiment. This is calculated taking into account the mean free path between particles pretended, the diameter of the particles involved and the scattering efficiency, which in turn depends on the incident wavelength and refraction indices.

The mean free paths chosen were 50000, 100000 and 200000 μm . This ensures, respectively, an average of 8, 4 and 2 particle interactions per travel. The volume fraction is given by equation C.1 in Annex C and represents the relation between the volume occupied by the microspheres and the volume of the smoke chamber, which in this case is a cylinder with known dimensions (400mm length, 50mm diameter).

Five experiments were conducted, the first four with single-diameter microspheres (1, 2, 3 and 6 μm) and a fifth one combining microspheres of different

Fig. 7.18.: Experimental setup.

diameters: $1\mu\text{m}$ (20%), $3\mu\text{m}$ (60%) and $6\mu\text{m}$ (20%). This last experiment tries to mimic the distribution of diameters of soot particles encountered in real smokes: they follow a lognormal distribution function and usually have very little soot content over $6\mu\text{m}$ [178, 173] –an exception is the case of oil smokes–.

Provided that the important parameter is the mean free path between radiation-particle interactions, the key parameter is the total number of microspheres n_t and the total volume of microspheres V_t (see Table 7.2 for a compilation of the resulting volumes):

$$n_t = n_{1\mu\text{m}} + n_{3\mu\text{m}} + n_{6\mu\text{m}} \quad (7.4)$$

$$V_t = V_{t,1\mu\text{m}} + V_{t,3\mu\text{m}} + V_{t,6\mu\text{m}} \quad (7.5)$$

The workflow for the experiments is as follows:

- The nebulizer is turned on, injecting the microspheres into the smoke chamber.
- Once the corresponding amount of aerosol and microspheres is inside, it is necessary to wait t_{evap} before making any measurements. In that moment, light is emitted and pictures are taken and saved for each radiating wavelength.
- Finally, the set is cleaned, recalibrated and prepared for the next experiment. Figure 7.18 shows an overview of the experimental setup.

Tab. 7.3.: Comparison between experimental and simulation setups.

	• Simulation	• Experiment
Optics	<i>Emitter:</i> 1x1 pixels @ 10 μ m <i>Receiver:</i> 320x240 @ 10x10 μ m <i>Noise Threshold:</i> -60dB <i>Time bins:</i> 100 <i>Wavelengths:</i> 476, 543, 623nm	<i>Emitter:</i> pinhole, 10 μ m <i>Receiver:</i> iPhone 6 camera, max 3264x2448 Raw data from sensor unavailable <i>Frame rate:</i> 240fps <i>RGB LEDs; Peaks:</i> 476, 543, 623nm
Media	<i>Particles:</i> suspended and still <i>MFP:</i> 50000, 100000, 200000 μ m <i>Setups:</i> 1, 2, 3, 6 μ m + mix 1-2-6	<i>Particles:</i> injection with nebulizer, suspension <i>MFP:</i> 50000, 100000, 200000 μ m <i>Setups:</i> 1, 2, 3, 6 μ m + mix 1-2-6
Geometry	<i>Chamber shape:</i> square section <i>Chamber length:</i> 0.4m	<i>Pipe:</i> circular section, 50mm diameter <i>Pipe length:</i> 0.4m
Contour conditions	<i>Temperature:</i> 25°C <i>Photon bundles:</i> 1e6	<i>Temperature:</i> 25°C -

Tab. 7.4.: Combination of variables for the experiments.

Variables		
Wavelength (nm)	Particle diameter (μm)	Mean Free Path (μm)
476 543 623	1.0	50000 100000 200000
	2.0	
	3.0	
	6.0	
	1.0 - 20%	
	2.0 - 60%	
	6.0 - 20%	

7.7. Results

A series of simulations was conducted, reproducing the experimental setup as closely as possible (see section 7.3) to be able to compare the results obtained by the simulations on the one hand and the experiments on the other hand.

A term-by-term comparison with the features of the real setup can be seen in Table 7.3. The incoming radiation beam (10 μ m vs. sizeless beam centered in a 10 μ m x 10 μ m pixel) and the chamber section (circular vs. square) are the most divergent settings. The chamber sections, given the chamber's diameter compared to the sensor size considered, do not have an impact in the overall results. However, the size and shape of the radiation beam may have a bigger impact and must be considered as a source for deviations between the simulations and the experimental results. The simulation results and their interpretation will be described first. Then, the experimental data will be presented, and experiments and simulations will be discussed last in Section 7.7.3.

Table 7.4 shows the combination of variables used for the experiments and the

Tab. 7.5.: Parameterization of the model for the simulations.

Case ID	Smoke type			Values obtained (simulation)	
	Particles	MFP (μm)	Wavelength (nm)	Max. Single-pixel power	Activated pixels
A1	6 μm $\odot$	50000	476	8.12e-11	3724
B1	1 μm $\odot$	50000	543	3.69e-10	198
C1	Mix (1-3-6 μm @ 20-60-20%)	50000	623	1.44e-10	479
A2	6 μm $\odot$	200000	476	5.56e-09	3873
B2	1 μm $\odot$	200000	543	2.05e-08	4204
C2	Mix (1-3-6 μm @ 20-60-20%)	200000	623	1.34e-08	4034

simulations. Given the amount of simulations and experiments run, only a small representative subset of the experiments and simulations conducted is shown in the Figures below.

7.7.1. Computer simulations

A total of 100000 photon bundles per simulation were launched. The tool presented in Section 6.5.1 was used to obtain information on the number and location of activated pixels at the sensor.

Six example cases were chosen among all those simulated. Their parameterization is shown in Table 7.5.

The dynamic range of the data obtained spanned over many orders of magnitude (the only limitation being the arithmetic capabilities of the computer); the sensitivity of a real sensor would be however much more limited. The simulation data obtained is displayed coloring the pixels where the radiation is received. A false color scale is used, from orange (maximum power at single pixel) to light blue (minimum value-noise threshold). Please note that false colors have nothing to do with the colors of the LEDs used in the experiments. The colors in the magnified subpictures at the bottom right corner of the pictures in Figure 7.19 and Figure 7.20 have been inverted for a better readout.

All activated pixels in those figures are marked in color, even the ones with levels under the noise threshold (which take a “minimum value/light blue” color). On the contrary, pixels not activated are displayed in black so that they are distinguished from activated pixels with very low received power. The “very low” or noise threshold has been fixed at -60dB in this case but can be configured to meet the dynamic range and sensitivity of the real sensor used². See Figure 7.21 for a comparison between the simulated data for a high sensitivity sensor and an iPhone sensor and the experimental results obtained.

The data visualization tool provides additional information on the time the photon bundle was received: by implementing time bins or intervals, it is pos-

²For comparison, the dynamic range of the naked eye spans over seven orders of magnitude, from 0.001 lux of a clear night sky to 100,000 lux of direct sunlight [294].

(a) Case A1 - Simulation.

(b) Case A1 - Experimental result.

(c) Case B1 - Simulation.

(d) Case B1 - Experimental result.

(e) Case C1 - Simulation.

(f) Case C1 - Experimental result.

Fig. 7.19.: Experimental results vs. simulation results for $MFP=50000\mu m$. The scale used in (a), (c) and (e) is a relative false color scale with a peak at 0dB (maximum - orange). Values under -60dB are marked as noise (minimum - light blue). The center of the images has been magnified and colors inverted in the bottom right corner, corresponding the minimum to reddish and the maximum to bluish colors.

(a) Case A2 - Simulation.

(b) Case A2 - Experimental result.

(c) Case B2 - Simulation.

(d) Case B2 - Experimental result.

(e) Case C2 - Simulation.

(f) Case C2 - Experimental result.

Fig. 7.20.: Experimental results vs. simulation results for $MFP=200000\mu m$. The scale used in (a), (c) and (e) is a relative false color scale with a peak at 0dB (maximum - orange). Values under -60dB are marked as noise (minimum - light blue). The center of the images has been magnified and colors inverted in the bottom right corner, corresponding the minimum to reddish and the maximum to bluish colors.

(a) High sensitivity simulation.

(b) Simulation using iPhone parameters.

(c) Real experiment with iPhone (zoomed).

Fig. 7.21.: Case B2: Comparison between a high sensitivity simulation with -60dB threshold, a simulation with iPhone parameters and the experimental result.

sible to link the amount of power received at a certain pixel location with its reception time frame. Although timing resolution was not validated at this time, the graphical tool is already prepared for the task.

Figures 7.22 and 7.24 show the accumulated power per pixel column and pixel row for the case B2 in linear or logarithmic scale respectively. The power value predicted at the central pixel is larger –by more than ten orders of magnitude or 100dB– than the values of the surrounding pixels. The power is concentrated in a narrow region around the center of the image (pixel with coordinates (160,120)).

7.7.2. Experiments

Following the criterion in the previous section, only the results of a small subset of the experiments conducted will be shown and commented. Taking case B2 again, Figures 7.23 and 7.25 show the accumulated power per pixel column and pixel row in linear or logarithmic scale as in the previous section. The original image was converted from color to grayscale and then to index (256 values) prior to obtaining the plots.

As the simulation predicts (see Figures 7.22 and 7.24), the power is concentrated in a narrow region. The peak obtained in the experiments is not coincident with the center of the image due to sensor misalignment. Image noise is in this case much more relevant than in the simulations. Values are around -1.5dB, although one must recall that the image has been processed and therefore quantitative comparison can only be made between images that have undergone the same process. In that sense, it has been observed that the values of “bright” pixels are between 10 and 20 times the values of dark, noisy pixels: index values of 100-200 for bright pixels are obtained (maximum index value is 255) for index values between 10 and 30 for noisy pixels. The fact that the bright region is very concentrated, along with the image size obtained by the sensor (3264x2448) and the quantization noise makes the image appear more noisy than it is in reality. It is interesting to observe that noise is not white, but increases towards the edges of the sensor.

The model allows the user to define a custom noise/detection threshold (sensor sensitivity). Defining a sensitivity closer to the one exhibited by the real sensor used in the experiments (an iPhone 6 in this case) and not marking the activated pixels below detection threshold in the simulations makes it possible to compare directly between simulations and results –at the cost of less information on the underlying physical processes–. Figure 7.21 shows this fact: the data obtained using the model with the iPhone settings in Figure 7.21(b) and the real picture obtained in the experimental setup in Figure 7.21(c) are almost identical. Given the sensitivity of the camera used and the experimental setups, it was decided to run the simulations at high sensitivity even if the results were no longer di-

(a) Number of columns = 320.

(b) Number of rows = 240.

Fig. 7.22.: Case B2 [Simulation]: Accumulated pixel power per column (a) and row (b) in linear scale.

(a) Number of columns = 2448.

(b) Number of rows = 3264.

Fig. 7.23.: Case B2 [Experiment]: Accumulated pixel power per column (a) and row (b) in linear scale.

(a) Number of columns = 320.

(b) Number of rows = 240.

Fig. 7.24.: Case B2 [Simulation]: Accumulated pixel power per column (a) and row (b) in logarithmic scale.

(a) Number of columns = 2448.

(b) Number of rows = 3264.

Fig. 7.25.: Case B2 [Experiment]: Accumulated pixel power per column (a) and row (b) in logarithmic scale.

rectly comparable and had to be interpreted: it is interesting not to lose that extra amount of information on the visualization screen.

Figures 7.19 and 7.20 show the results obtained for the other cases in Table 7.5, exhibiting a very good agreement between simulations and real experiments. Simulations predict the existence of a high power pixel in the middle of the picture along with some very low powered –reddish in the magnified subpictures– activated pixels around. Again, those pixels could not be detected by the camera sensor and consequently did not appear in the pictures (the bright central dot is clearly represented nevertheless).

The pictures obtained in the different setups are similar to one another. This does not mean in any way that the physical phenomena is the same. In fact, representing all the activated pixels, even those with very low powers, we wanted to state the differences between the simulation results for the different case setups and highlight their close agreement to Mie theory as an additional check.

In this first stage, interesting qualitative results were obtained. There is clear evidence of brighter (thus, more powerful) pixels for lighter smoke atmospheres (longer mean free paths); see cases A2, B2, C2 compared to A1, B1 and C1. Optical aberrations as well as emitter and sensor non-ideal behavior result in relatively bigger colored dots in the photograph (about 30-45 μm). Quantitative values can be obtained from the experimental data. However, due to the lack of information on the raw amount of power received at the sensor, only comparisons between different simulations on the one hand and between different experiments on the other hand can be made at this point.

7.7.3. Discussion and concluding remarks

The approach towards the validation of the smoke model presented here is generalistic and can be useful to validate other smoke models. A detailed description of the steps undergone and the generation of a reproducible, calibrated smoke has been described.

The first step towards the full validation of a modular smoke model that can be useful to simulate –in its more general concept–, interactions between incident electromagnetic signals and turbid media such as smoke has been presented. The model provides the user with an integrated simulation framework that includes: a physical emulation of the interaction between an incident signal and a single, defined particle, the aggregated smoke behavior, the description of the geometrical environment (including boundary conditions, description of emitter and receiver elements –pixels–, obstacles, objects, etc.) and a visual tool.

The use of event-based Monte Carlo simulations that incorporate timing data are highly valuable when it comes to performance assessment and rapid conclusions or design decisions. The validation of the timing capabilities has been left

out of this first stage, although its validation should be possible with a complementary setup.

The model proposed here can be easily applied to the simulation of a wide range of fire safety systems by feeding it with an adapted input and making the necessary changes to the geometry model. The configurable nature of the model proposed allows the user to simulate smoke types corresponding to different fire conditions with higher accuracy –by feeding more detailed scattering profiles, for instance– or use incident signals at other wavelengths. This fact can have positive implications on prototyping and early system development.

The results obtained so far are in close agreement with the simulations, providing at this point with qualitative validation data. In order to further assess the performance of the model, additional tests with more precise equipment such as advanced profile sensors capable of acquiring data in the submillisecond range would be necessary to conduct a full quantitative validation. However, it is possible to obtain quantitative data if two setups are compared.

The setups shown in the previous sections can help define the validity of the Mie approximation for real world smokes, obtaining statistical confidence values to employ when using that approximation to simulate real smokes with fractal-like particles. We believe this is an important step in the quest for devices to be used in low to no visibility environments.

8. Future work: trends and ideas

"Science never solves a problem without creating ten more."

George Bernard Shaw

This thesis has a number of research lines that can be seen as a natural follow-up of the work presented in the previous chapters. Several have been mentioned through the text but some of them can be highlighted:

1. A full qualitative validation including timing and special purpose hardware can provide with additional data to finetune and enhance the model.
2. The assessment of related and new conditions such as non-monochromatic illumination sources and more complex environment geometries, dispersive media with nonuniform distributions (particle concentration, size distribution) or other physical properties (temperature, etc.).
3. The validity of Mie analysis for real-world particles –including fractals at their different stages– can be also studied once the model has proven to be accurate with more controlled scenarios (spherical particles in the experiments and the simulations). The conclusions drawn from this study can serve know how rough the Mie approximation is for a given set of fire conditions. Conducting this study would be interesting as well for other environments for which the model has not been yet validated (haze, fog, turbid water, etc.).

Regardless of the number and importance of contributions that can be made with the aforementioned ideas, there are other major research lines that would be worth opening as they can help design new technologies and devices to overcome temporary vision impairment and so, bring the state of the art closer to the ultimate aim of this thesis. With this idea in mind, once the medium has been characterized in terms of propagation, the incoming signal must be exploited as much as possible, and in the most meaningful way.

The intrinsic features of the media considered alter the ongoing signals notably. It is thus necessary to tackle the problem using classical and novel views: in the recent times, new approaches to signal processing such as Compressed Sensing have emerged, forcing scientists and engineers to think outside the Shannon Theorem box. We believe that the applications using the work presented in the previous chapters will benefit from this new Signal Theory. Using it properly will

help us solve some of the challenges imposed by the degradation undergone by ongoing signals when propagating through harsh environments.

8.1. What if things were not quite as they seem?

After having their papers recurrently rejected by major journals, E. Candès, T. Tao and J. Romberg [295] on the one hand, and Donoho [296] on the other hand, finally managed to publish their work on “Compressive Sampling” or ‘Compressed Sensing (CS) back in 2006.

The main idea behind those groundbreaking papers is that against conventional wisdom, the sampling rate needed to acquire a signal can be much smaller than dictated by Shannon’s theorem (the Nyquist rate). To make this possible, the signal had to meet a number of requirements: it had to be *sparse in a certain basis*, and its sensing modality *incoherent*. Let’s see what these requirements mean:

- The idea behind **sparsity** is that if only some of the components of a certain signal contribute to the overall information carried by the signal, the effective information rate of that signal can then be much smaller than suggested by its Nyquist rate, and thus the signal can be compressed. For this to happen, one has to be able to find the basis under which the signal is sparse –that is, under which only few components of the signal carry most of its information– but still retain the information needed. This concept suggests that it may be possible to extract some kind of information –its useful part– while ignoring other kinds of information that could be present in the signal but are of little or no interest to our purposes: those “noninteresting” components will be close to zero in the appropriate basis. Complementary, sparse signals share a underlying, important feature inherent to CS: the information contained in the sparse signal has to be spread before arriving at the detector.
- The **sensing modality** makes reference to how we collect the data, and relates the “compressed” representation of the signal under the chosen basis with the “uncompressed” representation that occurs in the original domain in which they were acquired (time, frequency...). This may be seen as a generalization of the time–frequency duality that is now taken for granted and is of utmost importance for the problem discussed in the present work: the information spread in the components of the signal when represented in – for instance– time or frequency will be concentrated in some components when an adequate representation basis is chosen.

With these ideas in mind, one can say that compressed sampling is about extracting the *useful data* in a signal by choosing a *proper representation* of the signal. The ideas behind CS, disrupting as they are, have opened a whole new

field. Promising devices and technologies (around-corner imaging [149, 297], ghost imaging lidar [298], sensor networks [299]...) have been introduced and novel approaches to known problems (such as the one-pixel camera [300, 301]) have been suggested.

8.2. Compressed Sensing

Despite being in its infancy, Compressed Sensing (CS) has seen an enormous interest in the scientific community. With more than thousand research papers in about a decade, it is now an active field of research. There are a number of quality reviews and surveys on the topic for the interested reader. Some of them can serve as a good general introduction [302, 303, 304], while others focus on the theoretical aspects of compressed sensing [305, 306, 307]. There are also hands-on tutorials and code samples available online that help see compressed sensing in action [308].

A minimal introduction to CS will follow. The aim is not to give an overview of CS, but just to introduce the concepts that will be relevant when analyzing previous work and its implications within the scope of this thesis.

In general, the problem of sensing can be expressed in terms of a simple equation

$$Ax = b \quad (8.1)$$

where the features of object to be sensed x are extracted by means of a sensing matrix A yielding the measurement vector b . The problem facing CS is *how many measurements m do we need to acquire x exactly from b ? And approximately?*

The importance of these questions is clear: in a sense, it will depend on how “good” is our choice of A and how much information x has—in that basis—.

Algebra tells us that only if the number of measurements m is at least equal to the dimension of x (n), it will be possible to recover x exactly (determined or overdetermined problem). It is therefore important to obtain a good estimator for underdetermined problems. Hence, if x is sparse, that is, only S of its components are nonzero—i.e. it is “spiky” in that basis—, x will not be n -dimensional but S -dimensional in the basis. In principle, such signal would only need S measurements instead of n to be reconstructed perfectly at the cost of computation at the receiver end. In practice, most S -sparse signals can be recovered exactly once $m \leq 4S$ [309].

A first conclusion is that CS is advantageous when:

- Signals are sparse in a certain—known—basis.
- Measurements are expensive.
- Computations at the receiver end are cheap.

Fig. 8.1: l^1 minimization, the basis pursuit recovery algorithm for sparse signals. x^* is the value of x estimated in a noisy environment.

These premises apply to many fields, such as Magnetic Resonance Imaging (MRI) in medicine, astronomy or –our case–, imaging.

The computational load of CS is transferred to the *reconstruction* of the sparse signal. The simplest approach, an l^0 minimization is computationally intractable as it is not a convex optimization problem. However, l^1 minimization (basis pursuit) is convex and known to work well, see Figure 8.1 for a concept scheme. Recently, general optimization approaches for convex optimization have been published [310].

An important feature of compressed sensing recovery algorithms is that they can recover not only sparse signals x exactly but they can give approximate solutions x^* to compressible signals –signals approximately sparse– or noisy signals –see Figure 8.1(b)–. This result is important when turning theoretical systems into practical ones. Noise will not be further considered in the concept analysis undergone in this chapter.

Several **reconstruction techniques** have been put into practice such as *matching pursuit*, *iterative thresholding* or *model based* algorithms [311, 312, 313] with templates and specific software for convex optimization problems available as well [314, 315]. Near-optimal performance guarantees emerged in the 2000’s contributed by Candès-Romberg-Tao, Donoho, and others. Others have contributed with improvements to the subject of sparsity and sparse basis in CS, such as blind compressed sensing [316] or learning compressed sensing [317] that give alternatives when the basis under which the signal is sparse is not known *a priori*.

Another important result from the CS theory is the condition that **measurement matrices** have to meet. It is called *Restricted Isometry Property (RIP)* and

its demonstration is available in [305]. Interestingly, this property is obeyed by many types of matrices, notably by gaussian random matrices with high probability. For example, Walsh-Hadamard matrices meet the condition and have been widely used due to their mathematical properties, which make them convenient for CS.

The problem of CS can thus be divided into a measurement process and a reconstruction process: on the one hand, the measurement matrix (A in equation 8.1, commonly noted as Φ) must ensure that the information of an S -sparse signal is kept after the dimensionality reduction. On the other hand, the reconstruction must be as fast and as accurate as possible.

8.3. Related Work

In the recent years there has been an increasing interest and a growing number of practical systems relying on Compressed Sensing. Non-invasive medical imaging techniques such as MRI and ultrasound imaging have been among the first ones to benefit from CS [318, 319, 320] due to the great reduction that can be achieved in acquisition costs, even if it implies longer postprocessing times. Although primarily developed for biological tissues, most of the conclusions drawn can be extended to turbid (water) environments.

In the **imaging field** there are a number of research lines that are of significance and can be useful for applications in harsh environments. They all exploit the fact that natural or acquired images are usually *sparse* in nature. To name a few:

1. The study of *lenseless systems* able to recover the original phase function.
2. The use of CS techniques to reconstruct images using a *single detector* and far fewer samples than the original number of pixels in a given picture.
3. The use of *scatterers* with known transfer functions to mimic the use of a random sensing matrix.

A short review of the most important research lines will follow.

Using CS techniques, it is possible to remove lenses and thus the problem of blurring [321, 322]. Although an a priori knowledge of the complex transmission function of the diffuser is needed, they have the advantage of image reconstruction of static and dynamic objects. The method can be extended to image objects placed between thin scattering plates: this can be conceptually assimilated to an object embedded in smoke and remotely sensed.

Other authors have even taken advantage from the intrinsic randomness of scatterers as random sensing devices [323]. The drawback is, again, the need to calibrate the scatterer before making any measurements. If the scatterer does not change or is embedded in the device, the calibration can be made once at fabrication time.

Although focused on microscopy and diffraction tomography, it has been possible to obtain high quality depth resolved images using multi-wavelength phase retrieval and multi-angle illumination [324]. It can simplify the optical system through the use of a LED matrix, but requires long processing times.

Another approach is the use of wavefront shaping, which makes it possible to achieve perfect focusing through scattering media [325, 297].

The combination of natural scatterers with single-pixel detector is showing promising results [326, 327, 328]. They make use of phase retrieval algorithms [329].

In addition, using Hadamard measuring matrices in the form of low-intensity microstructured light patterns in combination with a single pixel detector (bucket detector), can serve to retrieve the image of a transilluminated object embedded inside highly diffusive material [330]. The bottleneck in this case is the switching speed of the Digital Micromirror Device (DMD) used, longer than the processing time. It is worth mentioning the “Single Pixel Camera” developed at Rice University [300], which was the first proof of concept of a single-pixel detector and has been since a milestone in CS imaging.

An interesting approach is given in [149] where imaging through scattering media is achieved combining the conservation properties of autocorrelation [331, 332, 333] and CS.

There are also alternative approaches to single pixel imaging with CS that take advantage of wavelets [334] to obtain adaptive resolution images with a bucket detector. Given the amount of postprocessing needed in this case, it is only interesting to obtain high-resolution images in still images, for example, in biological microscopy.

Single-pixel detectors combined with LIDAR and CS have shown great potential [335]. A number of authors have managed to obtain depth maps with good spatial resolution with single-pixel detectors [336, 337].

In [338], the authors demonstrate a real time video that combines visible and infrared images in real-time. To achieve this, they make use of high speed DMDs operated to obtain high resolution detail by arbitrarily modifying the DMD region of interest and mirror binning. In this case, each row from the Hadamard matrix, contains a different subset of spatial frequencies such that an $\sqrt{N} \times \sqrt{N}$ image can be fully sampled with N Hadamard patterns. This approach relies on sensing the light reflected in both outputs of the DMD (reflecting and non-reflecting), or alternatively, by displaying each pattern and immediately succeeding it by its inverse. In addition, using only the patterns whose measured signals yield “significant” magnitudes, a form of CS is applied. Hence, in this case, if the scene is static, this prediction can yield significant advances. We believe that the evolution of this predictive approach could lead to significantly cheaper SWIR imaging devices.

Last, it would be interesting to know if CS could improve or in some way bene-

Fig. 8.2.: Cases of study.

fit from recent advances in event cameras [339] or sub-wavelength reconstruction and resolution [340].

A coherent theoretical framework has to be developed and established considering all the constraints explained above in order to be able to set the basis for a feasible and robust imaging device.

8.4. Applications of CS for harsh environments

There are two cases of study that could benefit from the research advances presented above and that could be of special interest for harsh environments:

- A. An environment with minimum scattering, for example, a *lenseless thermal imaging* system. See Figure 8.2(a).
- B. A *remote sensing system* in a scattering environment (see Figure 8.2(b)).

As pointed out before, an important underlying condition of sparse signals that must be met for compressed sensing to work is the fact that the relevant information of the signal is contained in a few components if the signal is represented in a suitable basis but that information spreads across its samples, that is, there is a “random” deallocation of its relevant components. Therefore, there must be a physical mechanism that spreads that information. In the first case (Figure 8.2(a)), the lack of lenses and its consequent “blurring” of the image, and in the second case (Figure 8.2(b)) the scattering introduced by the medium itself, which will aggregate and spread the signal. Both mechanisms implement a sort of random sampling, which in turn serves to meet the RIP as presented in section 8.2.

Both cases may make use of the aggregation provided by single-pixel detectors.

Fig. 8.3.: Regular image vs. Sparse image.

8.4.1. Passive remote sensing system: lense-less IR system

Following 8.2(a), the received signal $I(\theta)$ can be expressed using convolution in the following terms:

$$I(\theta) = O(\theta) * S(\theta) \quad (8.2)$$

If, as said before, the scattering is considered to be negligible:

$$I(\theta) = O(\theta) * \cancel{S(\theta)} \approx O(\theta) \quad (8.3)$$

Here, the interesting advance that CS may provide is allowing the removal of the lenses of the IR camera. This could be significant for instance in FLIR cameras, where lenses are generally made of germanium due to their transmittance properties at the considered wavelengths (around 3-4 μ m). Germanium lenses account for most of the final price in these types of cameras. Issues such as speckle or the presence of artifacts should be considered carefully.

The use of one-pixel detectors¹, if the pair resolution-framerate can meet the specifications of a working system, could allow further weight and price reductions; always at the cost of increased signal processing or reduced speed and image quality. A key subject to consider is processing time, specially when aiming for responsive realtime applications such as video. In this case, processing time can be traded for resolution. With state of the art GPUs it is possible to obtain motion images at resolutions and framerates getting close to current FLIR cameras (320x240 pixels, 30-60 fps).

The advantage of CS in this case would be the integrability of these solutions (absence of lenses, one-pixel imaging) in helmets or other wearables. Mobility and weight are also benefited unless long operation times are needed; in this case battery size and weight would be an issue.

8.4.2. Active remote sensing system: LIDAR-like system

Again, the main idea behind compressed sensing is the exploitation of sparsity, which is a property naturally found in many signals (see Figure 8.3). For ex-

¹For instance, a single IR photodetector such as the one in [341].

ample, an original image can have detailed information on intensity, emissivity, temperature, or any other parameter such as time-of-flight.

For certain applications such as vision in compartment fires for trained staff, much of the information contained in a regular image may not be necessary. For example, there is no need to gather information about the color or exact material of the objects in a scene, but only their relative position and the overall framework is important. This fact makes it possible to remove a lot of unnecessary information from a certain picture and thus concentrate the information on a smaller set of relevant data. Indeed, it would be enough to obtain line images showing the contour of the objects in the compartment *approximately*, specially if the image is superimposed on a thermal image. Creative image generation schemes can be developed at that point.

In the case of LIDAR or other depthmaps, sparsity could come from images where an edge detection filter has been applied: the processed image would only show abrupt changes in distances (depths). Therefore, applying the Edge Detection Theory to the original depthmap recorded, the resulting image would be “sparser” in terms of the laplacian operator: $\Delta(\text{depthmap})$ [342, 343]. The sparser the signal considered, the better the general principles of compressed sensing will hold.

On the other hand, and irrespectively of the properties of the signals involved, the received signal at the sensor $I(\theta)$ can be expressed using convolution in the following terms (see Figure 8.2(b)):

$$I(\theta) = [E(\theta) * S(\theta)] * O(\theta) * S'(\theta) \quad (8.4)$$

Here, $E(\theta)$ and $I(\theta)$ are known. Applying the Fourier transform:

$$I(j\omega) = E(j\omega)S(j\omega)O(j\omega)S'(j\omega) \quad (8.5)$$

Which gives:

$$O(j\omega) = \frac{I(j\omega)}{E(j\omega)S(j\omega)S'(j\omega)} \quad (8.6)$$

In this case, if the scattering is minimum (for example, underwater imaging at relatively short distances), the equation above can be further simplified ($S(j\omega) \approx S'(j\omega) \approx 1$):

$$I(j\omega) = E(j\omega)O(j\omega) \quad (8.7)$$

$$O(j\omega) = \frac{I(j\omega)}{E(j\omega)} \quad (8.8)$$

The subject of image (and, more generally, signal) restoration has been an active subject of research with new algorithms and approaches being published regularly. The interested reader can find a good review on the subject in [344].

Fig. 8.4.: Propagation of the sensing signal. Autocorrelation.

8.5. Paving new ways for future developments

Honoring the memory effect described by Freund et al in [332], it has been shown that under certain conditions autocorrelation (C^{xx}) is preserved across scattering mediums (see section 8.3). In addition, the result of the Laplacian of the depthmap ($\Delta = \nabla^2$) –a well-known edge detection algorithm– is sparse. Taking into consideration the general signal processing analysis conducted in the previous section together with the sparsity of the “edge signal” ($C^{xx}(\nabla^2(\text{depthmap}))$) generated and the implications of the memory effect, it would be interesting to study possible emerging synergies.

Figure 8.4 shows the propagation of a sensing signal and its corresponding autocorrelation at every step. There the preservation of the autocorrelation would give $C^{x'x'} \approx C^{xx}$ and $C^{yy} \approx C^{y'y'}$. If the signal under consideration is sparse the process could further benefit from CS and open new ways for prospective applications.

In addition to the possibilities introduced by the use of CS techniques, it would be interesting to explore the benefits of combining different sensing modalities or types of signals. They could provide with more information on the environment sensed –if adequately exploited–, yielding significant synergies worth considering.

The questions raised above provide with enough elements to start new research lines, as they pose strong challenges for Physics, Mathematics, Signal Processing and Electronics, among other research domains. They are therefore open for discussion as future work.

9. Conclusions

“Stay hungry, stay foolish.”

Steve Jobs,
“Commencement speech,
Stanford University, 2005”

A doctoral dissertation is always a long and enduring trip never ready nor finished. This one is by no means an exception to that rule, with the long-term aim that served as an inspiration still active:

“To pave the way for future devices relying on remote sensing to present the users with artificially generated images that increase their situation awareness and thus their safety while conducting exposed tasks in smoke, turbid water or other particle-filled atmospheres”.

At this point of the journey, a series of significant milestones have been accomplished, getting us a step closer to the ultimate aim just stated. A number of side contributions have been arisen also along the way due to the multidisciplinary nature of the problem.

An in-depth analysis of the problem of temporary loss of vision in harsh environments and its consequences on spatial perception from a top level, system perspective has led to a subsequent analysis of the fundamental variables that take part on that process. As such, a basic (low-level) study of the properties and key factors of scattering from a signal propagation perspective has been conducted. In fact, the main contribution of this dissertation and its cornerstone is the modelization of particle-filled atmospheres. Some models treat smoke and other scattering atmospheres using macroscopic coefficients while others have focused on the interaction between an incident radiation and a single particle. Here, we have bridged that gap in some sense: making use of the computational power of GPUs, we could create a radiation propagation model at optical and infrared frequencies able to provide with macroscopic data aggregating individual particle-radiation interactions. This poses a truly challenging environment in the limit between Quantum physics, Electrodynamics and Thermodynamics.

The model has been designed with performance in mind: it has been implemented in a highly parallel architecture to minimize runtimes. A number of studies have been conducted on parallel code performance optimizations and practical conclusions have been drawn. An original instrument has been custom de-

signed and fabricated using state-of-the-art design techniques such as parametric design and additive manufacturing for full customization and cost-effectiveness. In addition, a first and promising step towards the validation of the model: highly correlated results have been shown, and the steps for a full quantitative validation have been pointed out.

The conclusions can be further expressed in line with the objectives in section 1.4 as follows:

1. On the definition of the research problem.

Understanding of the contour conditions and implications of the problem of temporary vision impairment needs a multidisciplinary approach. Many different scientific domains, from Psychology to Biology to Physics take part in the complex problem of perception. This fact makes it even more critical to define the research scope and its main aims as accurately as possible.

In this context, the definition of two *cases of study* has proven useful to bridge the theoretical problem of situation awareness in harsh environments to the need for a model of scattering media to aid in the design process of prospective technologies and devices.

2. On the study of previous research efforts.

Following the study of existing technologies and *state of the art devices*, the need to study the physics behind their mechanisms –from an engineering perspective– became clear. The study of wave theory and the similarities and differences between acoustic and electromagnetic waves, along with the *underlying physical processes associated to scattering* was important to define the possibilities and the approach to take depending on the application/medium considered. A deep understanding of the processes involved in the degradation of the signals when confronted with scattering media is key to the definition of successful systems.

3. On the definition of harsh media.

The *characterization of smoke* starting from the study of its composition and physical properties has made it possible to identify and define a set of parameters valid for a wide range of smoke types. This generalist approach would make it possible to analyze many other types of particle-filled atmospheres with little to no adaptation. The case of suspended sediments in water is one of them.

The separated analysis of the suspended particles from the atmosphere in which they are suspended was useful from a methodological as well as a conceptual point of view. It enabled the study of the relevant signal degradation mechanisms depending on the particular case, albeit with a systematic and hence more general approach.

4. On the creation of a model for the propagation of waves in scattering

environments.

Once different types of scattering media are systematized, a *model* can be developed. The model obtains data by aggregation using the Monte Carlo method. In other words, the model simulates the interactions between the incident radiation and a single particle, with the final result being the added consequence of the massive amount of interactions occurred.

The modular and scalable conception of the model has made it possible to create an *abstraction of the physical world* being simulated and so be able to simulate a wide scope of physical systems. The only requirement is that the definition of the environment and its contour conditions must be described using the standard set of parameters defined in the model.

The definition of the radiation-particle interaction is made at a *scale where neither quantum physics nor “macroscopic” electromagnetism hold well*. In our propagation analysis, elements from both worlds have been combined, with the corresponding mathematical analysis included in the text. It has the advantage of not needing to impose constraints to the type of medium considered, etc.

A battery of tests to assess the *self-consistency of the model*, plus a set of tests with different smoke types was conducted as a proof of concept. The results were discussed concluding with the good behavior of the model observed in terms of stability and data coherence.

5. On the implementation of the model and its performance analysis.

Given the computational demand of the model, its *eligibility to be implemented in a parallel architecture* was explored for performance reasons. The algorithm corresponding to the model was consequently implemented in a GPU.

In the quest for maximum performance, several implementations were tested and their performance compared. As a result, a simple set of rules was extracted to optimize the iteration process inherent to any performance optimization process involving implementations in GPUs using CUDA.

6. On the exploitation of the data provided by the model.

The amount of data the model can generate in a simulation can be huge. The exploitation of the data can easily *scale up to a big data problem*, since it is not difficult to obtain several GB's of data. However, it is not the amount of raw data but its quality what is important: a tool able to extract the useful information therein is necessary.

A *visualization tool* was developed in order to provide the user with a simple and intuitive way of extracting quantitative and qualitative data interactively. Improvements in exploitation tools can boost the perception of the quality of the model: the better the tool, the better the extraction of mean-

ingful data. In this sense, the development of an adequate presentation tool for the data generated should be considered from the beginning of the development process.

7. On the experimental setup to validate the model.

One of the most challenging tasks linked to any physical computer model is the validation of its results. In this thesis, an *instrument was designed and built* from scratch, with an innovative and rapid-prototyping design flow making use of advanced industrial design tools such as parametric design. This technology, combined with the use of additive manufacturing (3D printing) allowed to create a custom instrument in little time and at relatively low cost.

The experiments were designed to ensure the creation and preservation of a calibrated scattering medium at least while the measurements are made. This included dedicated hardware and some simple procedural optimizations to maximize throughput from each experiment.

The *fabrication and confinement of the scattering medium* is key. An original method to obtain a calibrated scattering medium (or *synthetic smoke*) was developed. The use of calibrated microspheres combined with a medical nebulizer made it possible to create the reliable and reproducible medium needed to compare the simulations with the experimental results.

Despite having tight budget and timing constraints, an excellent *qualitative correlation* between the simulations and the experimental results was observed. Simply changing the radiation source (for more power) and the sensor (for higher speed and sensitivity) would allow the obtention of the numerical data needed to conduct a full quantitative assessment –validation– of the model, which is left as future work. Timing data (arrival times) is provided by the model and could be assessed as well, although in this case a different instrumentation system would be necessary. Further measurements could even allow to assess the performance of the Mie approximation against real-world circumstances.

Finally, it could be interesting to explore the benefits of combining complementary sensing paradigms and advanced signal processing techniques such as *compressed sensing*. A number of preliminary results already published show high potential for some of the applications envisioned within the scope of this thesis.

We believe that we are now one step closer to the development of real mobile devices for artificial vision in particle-filled atmospheres.

Appendices

A. 3D Printed Parts: Plots

In this section, dimensioned technical drawings of the following items are included:

- Base holder.
- Intermediate holder.
- Inner cylinder.
- Linear holder for 25mm pipe.
- Square holder for 25mm pipe.
- Linear holder for 50mm pipe.
- Square holder for 50mm pipe.
- Flat holder.
- Microfilter holder and washer.
- EVA washer for the optical subsystem.
- Pipe ending with camera holder and nebulizer inlet.
- Pipe ending with optical inlet.
- Eccentric part for experiment optimization.

-

- **Intermediate holder.** Slightly asymmetric.

- **Inner cylinder.** It features a small pass-through hole in its upper part.

- Upper holder, linear for 25mm pipe.

- Upper holder, square for 25mm pipe.

- Upper holder, linear for 50mm pipe.

- Upper holder, square for 50mm pipe.

- Upper holder, flat.

- Microfilter holder and washer.

- EVA washer for the optical subsystem.

- Pipe ending with camera and nebulizer inlet.

- **Pipe ending** with optical inlet and excess air outlet (microfilter).

- Eccentric part and cover (which serves as PCB socket).

B. Instrumentation system: general overview

Next page shows the exploded view of the instrument designed for the scattering measurements. The numbers therein correspond to the following parts:

1. Optical bench.
2. Base holder.
3. Intermediate holder.
4. Inner cylinder.
5. Linear holder for 50mm pipe.
6. Sensor (digital camera).
7. Pipe ending with camera holder and nebulizer inlet.
8. 50mm diameter EVA washer (seal).
9. 400mm long, 50mm diameter high pressure PVC pipe.
10. 50mm diameter EVA washer (seal).
11. Microfilter holder and washer [1/2].
12. Microfilter: 47mm MILLIPORE 0.22 μ m membrane filter (GSWP 047 00).
13. Microfilter holder and washer [2/2].
14. 50mm diameter EVA washer (seal).
15. Pipe ending with optical inlet.
16. 20mm diameter EVA washer (seal).
17. 20mm long, 20mm diameter high pressure PVC pipe.
18. 25/20mm high pressure PVC pipe reduction.
19. 25mm high pressure PVC pipe socket.
20. 10 μ m pinhole, mounted (25mm diameter).
21. 25/20mm high pressure PVC pipe reduction.
22. 40mm long, 20mm diameter high pressure PVC pipe.
23. 20mm high pressure PVC pipe socket.
24. 40mm long, 20mm diameter high pressure PVC pipe.
25. 20mm diameter PCX lens.
26. Eccentric part for experiment optimization.
27. LED PCB with connectors.
28. LED PCB holder and cover.

C. Generation of calibrated synthetic smoke using microspheres

In this section, the method followed to create and inject calibrated synthetic smoke is described. Using monodisperse microspheres with known scattering diagrams and a desired mean free path distance between them it is possible generate controlled and reproducible smoke at a microscopic level.

Polystyrene microspheres exhibit high monodispersity, homogeneity and a uniform spherical shape, which makes them eligible for the validation experiments: no previous measurement has to be made for them, simplifying the overall process and avoiding sources of error. In addition, polystyrene is a convenient material: it is stable, inert, non-toxic and allows techniques such as vortexing or sonication of the microspheres without damaging or altering their geometrical shape.

There are several manufacturers that offer monodisperse microspheres of different sizes for research purposes which meet our requirements. Table C.1 summarizes the main characteristics of the commercial microspheres that were used for the experiments. The complex refractive indices of the spheres necessary for the model have been extracted from [345] for the corresponding wavelengths.

The spheres must undergo certain processes to be effectively suspended in the particle chamber. The method to ensure that the two key properties of the particles in the medium are met (average mean free path between particles and known optical properties) is described in the following sections. The rest of the parameters such as air temperature and refraction index are easily determined.

Tab. C.1.: Main characteristics of the commercial suspensions of polystyrene microspheres used in the validation experiments.

Brand	Model	Nominal diameter (μm)	Coefficient of Variance (%)	Solid content (%)
Ikerlat Polymers	AJ-1000	1	<0.5	10
Polysciences	19814-15	2	5	2.5
Polysciences	17134-15	3	5	2.5
Sigma-Aldrich	89756-5ML-F	6	<2	2

Tab. C.2.: $\Psi = \frac{2d}{3Q_{sca}}$ as a function of wavelength and microsphere diameter.

Lambda vacuum (nm)	d = 1μm	d = 2μm	d = 3μm	d = 6μm
395	2.24E-007	6.41E-007	8.17E-007	1.99E-006
476	3.61E-007	5.36E-007	8.09E-007	1.76E-006
543	3.20E-007	6.21E-007	9.88E-007	1.81E-006
623	2.23E-007	5.10E-007	7.90E-007	1.75E-006
730	1.66E-007	4.99E-007	1.01E-006	1.67E-006
890	1.50E-007	6.61E-007	7.95E-007	1.73E-006

C.1. Amount of particles in the simulation chamber

The diameter and length of the pipes used for the experimental setup determine the volume of the simulation chamber and indirectly the number of microspheres needed for a target mean free path between them. From Section 5.3.1, we have that the volume fraction of microspheres ϕ is expressed as:

$$\phi = \frac{2d}{3Q_{sca}\Lambda_{(MFP)}} \quad (C.1)$$

where d is the diameter of the microsphere, $\Lambda_{(MFP)}$ the mean free path between microspheres and Q_{sca} the scattering efficiency. Using the software provided by Scott Prahl in [113], it is possible to obtain a table containing the values for $\frac{2d}{3Q_{sca}}$ as a function of wavelength and microsphere diameter; see Table C.2.

Naming $\Psi = \frac{2d}{3Q_{sca}}$ gives the following expression for the volume fraction:

$$\phi = \frac{\Psi}{\Lambda_{(MFP)}} \quad (C.2)$$

Equation C.2 and Table C.2 make it possible to find the volume fraction of the microspheres as a function of the mean free path in microns, which is related to the mean number of interactions between the incident radiation and the microspheres. Table C.3 shows values of the volume fraction for different values of $\Lambda_{(MFP)}$.

Once the desired mean free path has been set and the volume fractions computed for the particular size of the microspheres in the experiment, the next step is to decide the simulation volume. In principle, the bigger the volume, the better, as there is less chance for spurious interactions with the walls of the simulation chamber. The high cost of the microspheres used in the measurements condition the amount of spherules per test and thus the volume of the simulation chamber for a given volume fraction.

As an example, for a mean free path of 100000μm (10cm) and a 1m long, 50mm diameter pipe illuminated at 395nm, the amount (volume) of 1μm microspheres

Tab. C.3.: Volume fraction of microspheres as a function of wavelength, microsphere diameter and mean free path.

Lambda vacuum (nm)	d = 1 μm		
	$\Lambda_{(\text{MFP})} = 50000\mu\text{m}$	$\Lambda_{(\text{MFP})} = 100000\mu\text{m}$	$\Lambda_{(\text{MFP})} = 200000\mu\text{m}$
395	4.47E-006	2.24E-006	1.12E-006
476	7.21E-006	3.61E-006	1.80E-006
543	6.40E-006	3.20E-006	1.60E-006
623	4.45E-006	2.23E-006	1.11E-006
730	3.33E-006	1.66E-006	8.32E-007
890	3.00E-006	1.50E-006	7.51E-007
Lambda vacuum (nm)	d = 2 μm		
	$\Lambda_{(\text{MFP})} = 50000\mu\text{m}$	$\Lambda_{(\text{MFP})} = 100000\mu\text{m}$	$\Lambda_{(\text{MFP})} = 200000\mu\text{m}$
395	1.28E-005	6.41E-006	3.21E-006
476	1.07E-005	5.36E-006	2.68E-006
543	1.24E-005	6.21E-006	3.11E-006
623	1.02E-005	5.10E-006	2.55E-006
730	9.98E-006	4.99E-006	2.50E-006
890	1.32E-005	6.61E-006	3.30E-006
Lambda vacuum (nm)	d = 3 μm		
	$\Lambda_{(\text{MFP})} = 50000\mu\text{m}$	$\Lambda_{(\text{MFP})} = 100000\mu\text{m}$	$\Lambda_{(\text{MFP})} = 200000\mu\text{m}$
395	1.63E-005	8.17E-006	4.08E-006
476	1.62E-005	8.09E-006	4.05E-006
543	1.98E-005	9.88E-006	4.94E-006
623	1.58E-005	7.90E-006	3.95E-006
730	2.02E-005	1.01E-005	5.05E-006
890	1.59E-005	7.95E-006	3.98E-006
Lambda vacuum (nm)	d = 6 μm		
	$\Lambda_{(\text{MFP})} = 50000\mu\text{m}$	$\Lambda_{(\text{MFP})} = 100000\mu\text{m}$	$\Lambda_{(\text{MFP})} = 200000\mu\text{m}$
395	3.98E-005	1.99E-005	9.95E-006
476	3.51E-005	1.76E-005	8.78E-006
543	3.61E-005	1.81E-005	9.03E-006
623	3.50E-005	1.75E-005	8.76E-006
730	3.34E-005	1.67E-005	8.35E-006
890	3.45E-005	1.73E-005	8.63E-006

necessary would be:

$$V_{\text{spheres}} = V_{\text{pipe}} \cdot \phi = \pi r^2 h \phi = \pi (25 \cdot 10^{-3})^2 \cdot 1 \cdot \phi \Big|_{\frac{395 \text{ nm}}{100000 \mu \text{ m}}} =$$

$$= \pi (25 \cdot 10^{-3})^2 \cdot 2.2410^{-6} = 4.4 \cdot 10^{-9} \text{ m}^3 = 4.4 \cdot 10^{-3} \text{ cm}^3$$

$4.4 \cdot 10^{-3} \text{ cm}^3$ of dry polystyrene microspheres, which correspond to 0.176ml of 2.5% solid volume suspension.

Once the amount of microspheres to be fed has been calculated following the procedure described above, the next issue is to suspend the microspheres in the smoke chamber so that they remain stable for the time needed for the experiments and do not aggregate. This last requisite is important, as aggregation would cause the geometries to change, resulting in different scattering profiles and yielding measurements that would not match those simulated.

All the acquired suspensions are aqueous. Some kind of surfactant is also added to prevent aggregation during storage or transportation. Therefore, there is a need to design a method to make an aerosol from the latex containing the microspheres. It is necessary to grant that the microspheres do not aggregate and that, simultaneously, the aerosol carries them inside the medium chamber. Once there, the liquid phase of the aerosol (acting as a carrier) must evaporate, leaving the dry homogeneous microspheres suspended as still as possible during the experiments.

C.2. Particle carrier and nebulation evaluation

It is clear that water –where the commercial microspheres are originally suspended– is not a good carrier, as the time it takes for water to evaporate is longer than the settling time of the microspheres. Other carriers must be examined, taking into account the wanted features: high volatility and stability, non-solvent of polystyrene and easy to manipulate. Studying the solvent listing in [346], the final candidates are: ethanol and methanol.

In order to assess the best carrier for the microspheres, a set of tests were conducted. The aim was to identify the time intervals where the experimental data can be obtained in the best conditions.

Figure C.1 shows the ideal time line with the most relevant time milestones to be identified during the carrier evaluation experiments. At $t = 0$ the nebulization is started. The aerosol reaches the end of the pipe (smoke chamber) and fills it at t_{full} . t_{nebul} is reached when the solution has been completely nebulized and all the microspheres are in the chamber. The carrier is evaporated t_{evap} after t_{nebul} . From that moment on, the smoke is stable and pictures can be taken for a period of t_{stable} . An important moment is where the atmosphere gets saturated and droplets start to appear. This happens at t_{droplet} and is not a desirable situation. Therefore,

Fig. C.1.: Time line for nebulization and ideal time interval for the experiments (t_{exp}).

the ideal time frame to conduct the experiments t_{exp} is between $t_{\text{nebul}} + t_{\text{evap}}$ and t_{droplet} :

$$t_{\text{exp}} = \begin{cases} [t_{\text{nebul}} + t_{\text{evap}}, t_{\text{nebul}} + t_{\text{evap}} + t_{\text{droplet}}], & \text{if } t_{\text{droplet}} \leq t_{\text{nebul}} + t_{\text{evap}} + t_{\text{stable}} \\ [t_{\text{nebul}} + t_{\text{evap}}, t_{\text{nebul}} + t_{\text{evap}} + t_{\text{stable}}], & \text{otherwise} \end{cases} \quad (\text{C.3})$$

Using the notation above, the ideal aerosol would have the following characteristics:

- Uniform filling.
- Low t_{nebul} .
- Very short t_{evap} .
- High stability: long t_{stable} .
- No droplet formation or very long t_{droplet} .

Times defined above depend largely on the droplet sizes of the aerosol carrying the microspheres as well as on the carrier chosen (ethanol or methanol). The smaller the droplets, the easier it will be (shorter times) to evaporate the carrier. This means that droplets bigger but close to particle sizes are more efficient: the amount of liquid carrier per droplet to evaporate would be smaller this way.

The PARI LC nebulizer presented in section 7.3.4 is well suited for the nebulization task. It is designed for the medical praxis and therefore it must generate uniform atmospheres.

With all of the above elements it is now possible to characterize ethanol and methanol in order to evaluate the best carrier for the validation setup. The measurements were made under the following variables:

- Possible carriers: ethanol and methanol.
- Nebulizers - droplet size: 2, 3 and $7\mu\text{m}$.
- Connectors and pipes: free (no smoke chamber, where applicable), 25mm diameter pipe (400mm and 1000mm length) and 50mm diameter pipe (400mm and 1000mm length).

A transparent PVC pipe was used for these tests, as that way it was possible to see the quality and stability of the whole process. The pipes and the nebulizers

were cleaned and dried after each experiment.

The times measured are further defined as follows:

- t_{full} : time passed from the beginning of the nebulization to the moment the aerosol starts to pass through a small aperture left to prevent overpressure at the other end of the pipe. Results are summarized in Table C.4.
- t_{nebul} : time passed from the beginning of the nebulization to the moment where no aerosol is seen coming from the nebulizer for 2 seconds. (Note: when little or very little suspension is left in the nebulizer, nebulization starts to be intermittent. An interval of 2 seconds is a good trade-off between time and amount of nebulized suspension.) Results are presented in Table C.5.
- $t_{droplet}$: time passed from the beginning of the nebulization to the moment where droplets start to appear. They start to appear in the lower part of the pipe, close to the nebulizer inlet. The moment where droplets appear mark the end of effective nebulization and so, a qualitative result suffices, however the results are available in Table C.6. In fact, in all cases $t_{droplet} < t_{nebul}$ for ethanol, while the contrary, $t_{droplet} > t_{nebul}$, held true for methanol. This result would justify by itself the use of methanol, as ethanol droplets are formed very early, while methanol did not form any. The explanation could be due to differences in vapor pressure of ethanol as compared to methanol. At 20°C ethanol's is 5.95 kPa, while methanol's vapor pressure at the same temperature is 12.8 kPa.
- t_{evap} : time passed from the moment the compressor is stopped (t_{nebul}) to the moment where the aerosol cannot be seen. Results are summarized in Table C.7.

An analysis of the data presented in Tables C.4-C.7 reveals an important behavioral gap between 2-3 μ m and 7 μ m particles. Bigger ones have shorter nebulization times due to higher liquid throughput (more volume per sphere). Evaporation times are about the same for all three particle sizes. The only anomaly appears for 7 μ m particles in 1000mm, 50mm $\varnothing$ pipes, which exhibits certain aerosol for longer.

The only worrying result is $t_{droplet}$ for 7 μ m particles, as it is shorter than t_{evap} . This can have an impact in the results obtained experimentally when compared to those computed using the model. Nevertheless, even if droplets are present, for the case of methanol the amount of droplets is very small and does not tend to grow significantly over time. In fact, several techniques such as mildly heating the pipe could prevent drop formation. The experiments will be run following the general procedures, taking into account that the existence of droplets can be an error source.

Stability is an important issue as well because the synthetic smoke must meet the quasi-static approach during the time needed to take measurements: in this

Tab. C.4.: t_{full} in seconds as a function of droplet size and pipe type.

	Droplet size	Pipe configuration (diameter, length in mm)			
		25 $\varnothing$, 1000	25 $\varnothing$, 400	50 $\varnothing$, 1000	50 $\varnothing$, 400
Methanol	3 μ m	3.80	1.50	- (1)	7.06
	4 μ m	3.40	1.56	- (1)	5.89
	7 μ m	3.50	1.56	15.00	4.98
Ethanol	3 μ m	3.80	1.70	14.90	4.96
	4 μ m	3.40	1.61	14.50	4.48
	7 μ m	3.80	1.61	19.20	5.11

(1) Unable to determine. Very faint.

Tab. C.5.: t_{nebul} for 2ml of carrier in minutes:seconds as a function of droplet size and pipe type.

	Droplet size	Pipe configuration (diameter, length in mm)				
		No pipe	25 $\varnothing$, 1000	25 $\varnothing$, 400	50 $\varnothing$, 1000	50 $\varnothing$, 400
Methanol	3 μ m	3:35	3:48	3:40	3:25	3:20
	4 μ m	3:30	3:45	3:46	3:57	3:49
	7 μ m	1:56	1:46	1:49	1:47	1:47
Ethanol	3 μ m	4:50	5:04	4:52	4:56	4:37
	4 μ m	4:28	4:45	4:39	4:50	4:30
	7 μ m	2:44	2:45	2:46	2:45	2:47

Tab. C.6.: $t_{droplet}$ in seconds as a function of droplet size and pipe type.

	Droplet size	Pipe configuration (diameter, length in mm)			
		25 $\varnothing$, 1000	25 $\varnothing$, 400	50 $\varnothing$, 1000	50 $\varnothing$, 400
Methanol	3 μ m	-	-	-	-
	4 μ m	-	-	-	-
	7 μ m	<10	<15	<20	<20
Ethanol	3 μ m	-	-	-	-
	4 μ m	-	-	-	-
	7 μ m	<10	<10	<20	<20

Tab. C.7.: t_{evap} in seconds unless otherwise stated as a function of droplet size and pipe type.

	Droplet size	Pipe configuration (diameter, length in mm)			
		25 $\varnothing$, 1000	25 $\varnothing$, 400	50 $\varnothing$, 1000	50 $\varnothing$, 400
Methanol	3 μ m	15	6	16	40
	4 μ m	9	7	37	45
	7 μ m	15	18	>3 min	40
Ethanol	3 μ m	>3 min	>3 min	>3 min	>3 min
	4 μ m	>3 min	>3 min	>3 min	>3 min
	7 μ m	>3 min	>3 min	>3 min	>3 min

case, a picture (4ms with the iSight camera in slow motion mode). With the available equipment it was not possible to analyze the movement of individual particles in that time interval. However, the atmospheres created exhibited high degree of stability with naked eye observations, maintaining their properties (buoyancy, density, etc.) for several minutes in many cases, specially in the case of smaller particles. More complex setups to measure and monitorize the aerosol (using Doppler, for instance) are not justified at this point.

C.3. Preparation of the particles

The experiments in the previous subsection show that the best carrier to use for the validation is methanol. It is therefore necessary to make a phase change, from the aqueous solution in which the microspheres are delivered to methanol. Table C.1 shows the characteristics of the commercial solutions used, with preparations varying from 2 to 10% solid content.

The phase change procedure is gradual and inspired in [347, 348]. It is included here for completion:

1. The suspension supplied (100% water) is vortexed.
2. The sample is centrifugated at 10900rpm for 2 minutes.
3. The supernatant is then removed, with caution to avoid removing the microspheres at the bottom.
4. New solvent is added at this point: 75% water, 25% methanol. Steps above are then repeated, adding solvent with increasing methanol concentrations: 50% water, 50% methanol, 25% water, 75% methanol and finally 100% methanol.

Once the suspension in pure methanol has been obtained, it is important to prevent evaporation before the experiment is actually conducted. One option is to use parafilm to seal the Eppendorf wells used with the methanol suspensions and keep them refrigerated at 2-8°C. It is convenient to circumvent the phase change process to the immediate amount needed for the experiments, leaving the rest in water for long term storage (also refrigerated at 2-8°C). It is necessary to prevent freezing, as the agglomeration resulting is not reversible by any normal means (sonication, vortexing, etc.).

The possibility of vortexing without affecting the quality of the microspheres to eliminate any form of aggregation is an advantage of the use of polystyrene as it is fast, easy and effective. Other techniques can also be used, such as sonication. To ensure the correct behavior of the microspheres during the experiments, a microscope preparation was done prior to nebulization to ensure there was no aggregation. Figure C.2 shows microspheres before and after phase change and vortexing.

Fig. C.2.: Impact of vortexing on the aggregation of microspheres (Ikerlat AJ-1000).

C.4. Injection of the particles in the medium chamber

Once the suspension of the microspheres in the appropriate carrier has been obtained, the next step is to feed that suspension into the smoke chamber for measuring. See section 7.3.4 for more details on the process.

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