Developing Software to Connect Aerodynamic and Microscopic Measurements on Soot Particles

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Objective

The project has built a software package for researchers to analyze the optical properties of soot particles with complex shapes. The main focus was to link laboratory data with executable parameters for a soot modeling software to generate appropriate sample soot aggregate for soot optical property simulations.

This project

- aids climate researchers by improving the quality of available tools
- advances our knowledge on climate change
- contributes to education activities at the University of New Haven
- raises environmental awareness among students

A converter was built to convert laboratory measurement data (particle mobility size, mass and/or effective density) into practical parameters input information [number of primary spheres, fractal dimension (or its equivalences), and dynamic shape factor, etc.]. These inputs are then used in an modified open-source soot modeling software, Modified FracMAP to generate model fractal soot aggregates that simulate the aforementioned property parameters. The end-users may then use the model soot aggregates for light scattering and absorption simulations, using available software packages such as ADDA and DDSCAT.

Figure 1.1: A Flowchart showing the organization of our software package that converts experimental results into sample soot aggregates for soot optical property simulations.

Background

Soot is generated during the incomplete combustion of fossil fuels and wildfires. Soot particles are very complex in shape: they exist as an aggregate of tiny spheres (10-50 nm in diameter) that are made of pure elemental carbon (EC). EC is very efficient at absorbing the infrared spectrum of solar radiation. This contributes significantly to climate change by retaining the incoming solar energy. In geographic locations with significant soot emissions, including many megacities worldwide, radiative heating by soot is comparable to that by the greenhouse gases. Thus, an accurate evaluation of the optical properties of atmospheric soot is crucial to allow better climate predictions.

One approach to investigate optical properties of soot is to determine them experimentally. For example, by using special instrument called nephelometer, soot particles are subjected to a strong beam of light at specific wavelength and also record light intensity which is scattering away by soot.

Alternatively, numerical model have been develop based on physical and chemical principle to simulation optical properties of soot particles. Major challenges in these simulations are (1) the lack of direct correlation between lab results and computer modeling inputs and (2) the complex morphology of soot particles. Here, morphology refers to the configuration of these EC spheres mentioned above. Soot has a fractal morphology as shown in *Figure 1.3* with many irregular branches and splits and may be described using a pre-factor (k_g) and fractal dimension (D_f): $number\ of\ EC\ spheres = k_g (size)^{D_f}$, where size of the aggregate is defined as the ratio between the radius of gyration and the diameter of the EC spheres.

Iterative Development Process

- 1) Established program requirements with the client that this program needed to meet.
- 2) Worked with client to determine program behavior and acquire the relevant formulas.
- 3) Develop pseudo code that implements the formulas and algorithms.
- 4) Build a prototype that implements the pseudo code.
- 5) Test the prototype results against expected theoretical results to verify accuracy.

The converter is a predominantly Python application that offers the user multiple input options based on their experimental conditions, as shown in *Figure 1.2*. The open-source FracMAP was significantly modified to adapt it to our needs (*Figure 1.3*). 3D modeling software, Babylon.JS, helped us to quickly check that the result looked as we expected from a qualitative standpoint as seen in *Figure 1.4*. A dipole generator was also developed to interface the modified FracMap results (error analysis on the accuracy of our dipole generator was shown in *Chart 1.1*.) and the open-source ADDA software.

Figure 1.2: The user interface of our converter with various input options for users to calculate parameters of soot particles based on their experimental results.

Figure 1.3: A screenshot of our modified version of FracMAP generating a fractal aggregate based on a set of given parameters. After this model is generated our algorithm breaks the nanospheres into smaller spheres called dipoles for further ADDA simulation on soot optical properties.

Figure 1.4: External modeling tools such as Babylon.JS were used to quickly verify that the algorithm results look as expected. Above is a model that was transposed.

Results and Discussion

Chart 1.1: The chart displays the errors between the expected results that came from the premade bi-sphere shape in ADDA with the dipoles that were generated by our algorithm. As the number of dipoles increased, so did the accuracy.

Errors of Dipole Generation Algorithm		
Number of Dipoles Used	Extinction	Absorption
36	58.0220%	57.5409%
195	0.8626%	0.8625%
23,857	0.0606%	0.0614%
190,833	0.0259%	0.0257%
1,526,410	0.0679%	0.0673%
23,856,411	0.0041%	0.0041%

Our software products are open source software packages available through the following links:

- (1) Converter: <https://github.com/Naneis-wyx/Fractal-Aggregate-Convertors-Sub>
- (2) Modified FracMap and Dipole Generator: <https://github.com/Christopher-Hayes/mfm>

Challenges

Testing Complex Aggregates

Since there isn't any other readily available software that also analyzes light scattering and absorption on complex aggregates that take nanosphere overlap into account, we didn't have a benchmark to compare our data with. Our core testing was done with basic shapes that could be reproduced without our algorithm.

Working with Various Open-Source Programs

Our software package boths builds on open-source programs and works in-between distinct software programs. This provided us with the challenges of needing to be able to build on software that was already built, such as FracMAP in C++, as well as develop our own solution in Python that can interface with FracMAP.

Research-Heavy Computer Science Project

This project was a little more challenging than the traditional implementation focused project because of its research component. Working with the software required a basic understanding of the chemistry of soot aggregates. Implementing solutions often involved working with formulas. Quick prototyping followed by testing and often implementation changes based upon feedback from testing played an essential role in this project.

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