SoftwareX

SootLib: a soot model library for combustion simulation

--Manuscript Draft--

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Abstract:	Soot formation in combustion is an important process that affects radiative heat transfer, flame temperatures, and emissions with health and environmental impacts. Soot formation involves complex chemistry for nucleation, growth, oxidation, and coagulation processes. The soot particles vary widely in size and accurate modeling requires representation of the particle size distribution (PSD). Modeling soot is not trivial, and is only one of several physical processes active in combustion systems. This paper presents a software package called SootLib, which is an open-source library for modeling soot formation and other aerosol systems. SootLib is written in C++, is documented with Doxygen, and is available on GitHub. The library includes several models for soot chemistry and coagulation, and it represents the PSD using either a sectional model or the method of moments (MOM). Four closure approaches for the MOM are implemented allowing up to eight moments: monodispersed, an assumed-shape lognormal distribution, the quadrature method of moments, and the method of moments with interpolative closure. SootLib provides an interface for inclusion in other combustion packages including CFD or reacting flow solvers. The range of of models allows comparisons and sensitivity studies, and the modularity facilitates extension to other soot models.
Suggested Reviewers:	Tony Saad, PhD Assistant Professor, University of Utah tony.saad@utah.edu Expert in reacting flow simulations for which this submitted software is intended.
	Randy McDermott, PhD Principal Developer, National Institute of Standards and Technology randall.mcdermott@nist.gov Randy is a principal developer of the Fire Dynamics Simulator (FDS) code. Soot is a major component of fire simulation and could be used with a code like that submitted here.

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Figure

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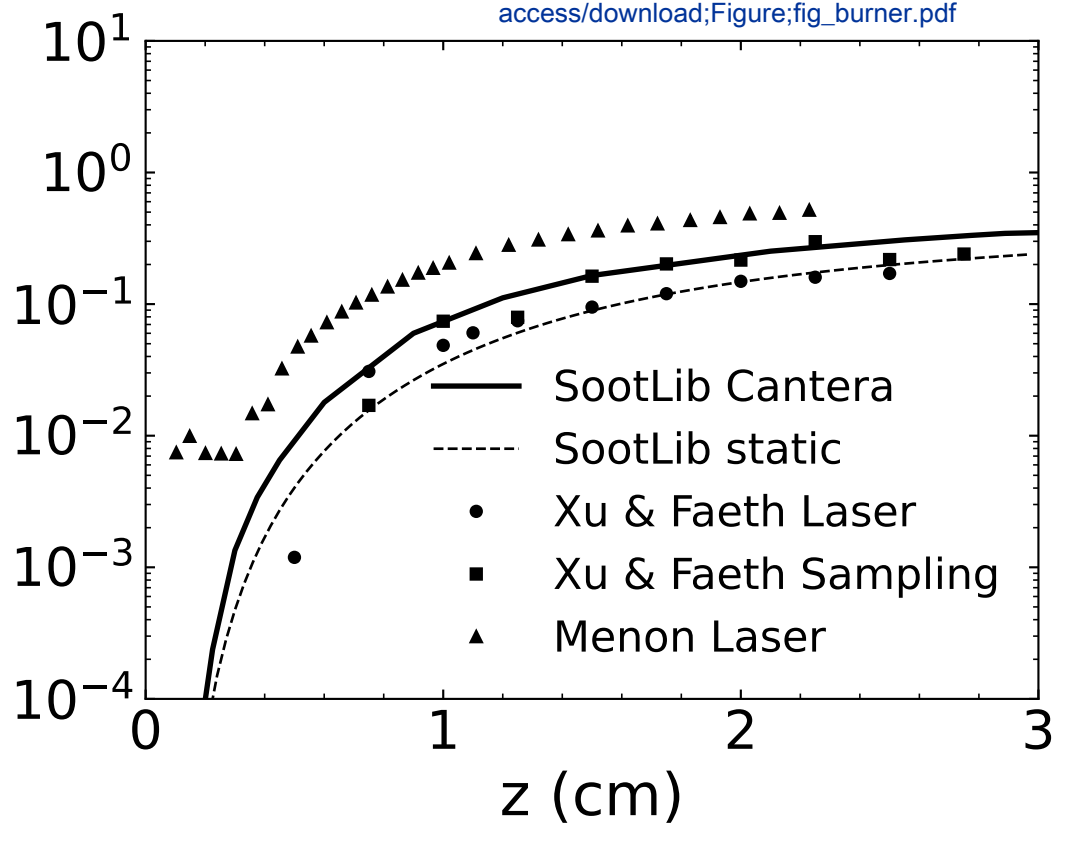

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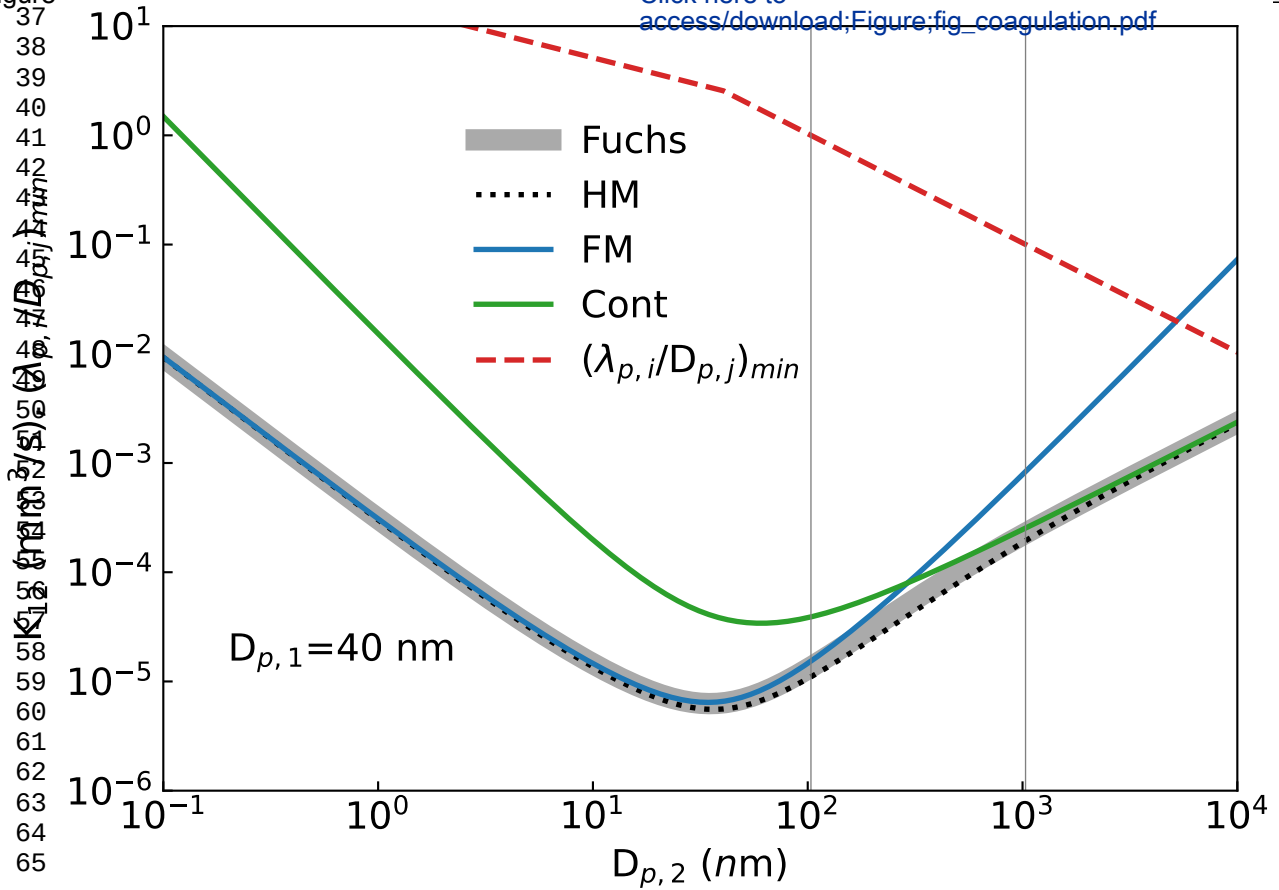

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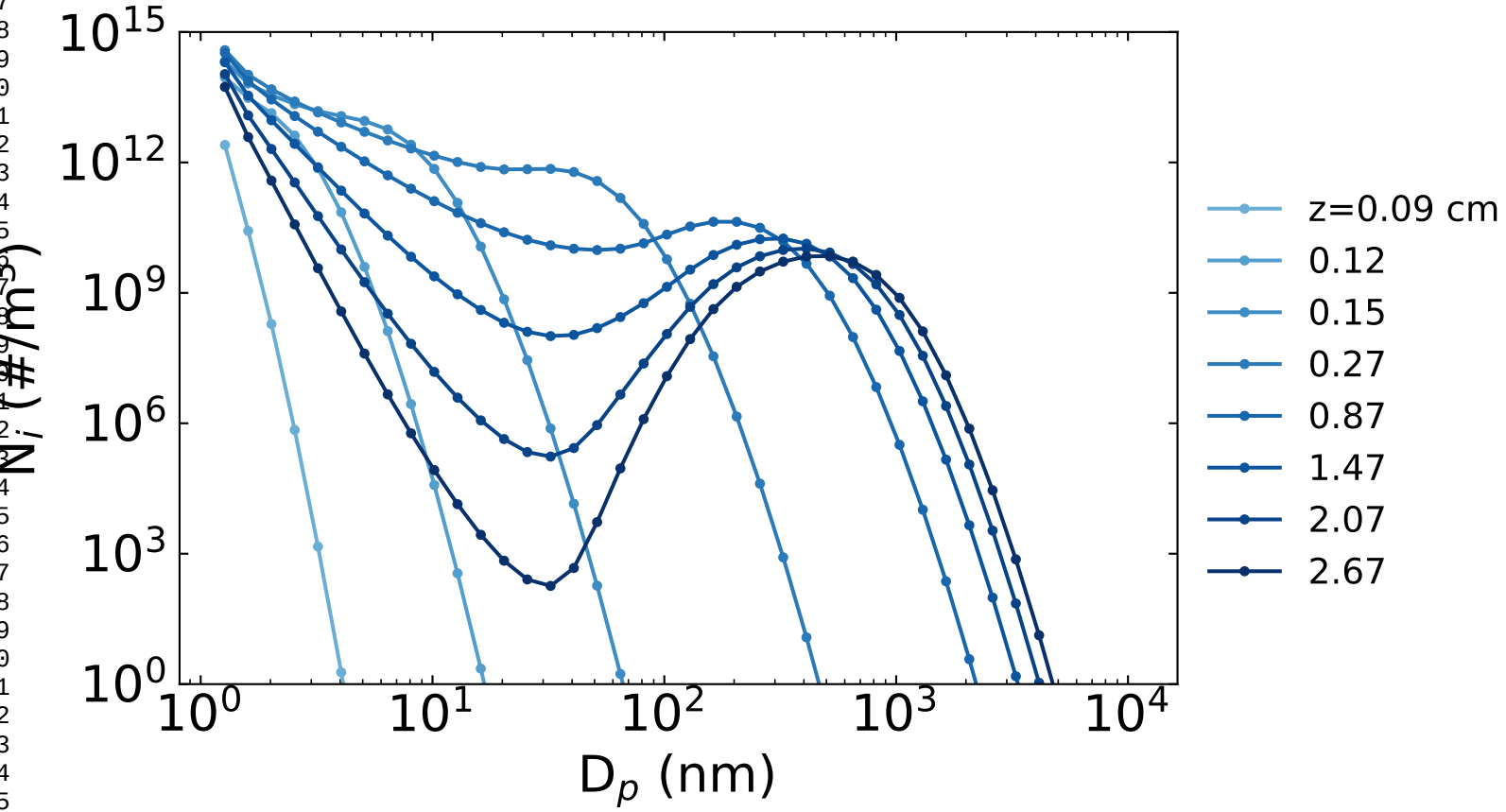

Conflict of Interest Declaration

There are no known conflicts of interest associated with this publication and there has been no significant financial support for this work that could
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