Pacific Northwest NATIONAL LABORATORY

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Modeling particulate generation during high energy explosive events

September 2021

Manish Shrivastava
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U.S. DEPARTMENT OF ENERGY

Prepared for the U.S. Department of Energy
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Introduction

Laser produced plasmas are used to simulate high energy events and are useful for a variety of applications e.g. in industrial sectors, such as semi-conductor manufacturing, as well as medical, environmental, and energy sectors. Particulate generation in laser produced plasmas is related to key features of the plasma: temperature and pressure evolution during plume expansion, plasma chemistry etc. Several uncertainties persist in relating initial high energy events (~microseconds) to particulate formation that happens as the plasma cools and evolves (~milliseconds).

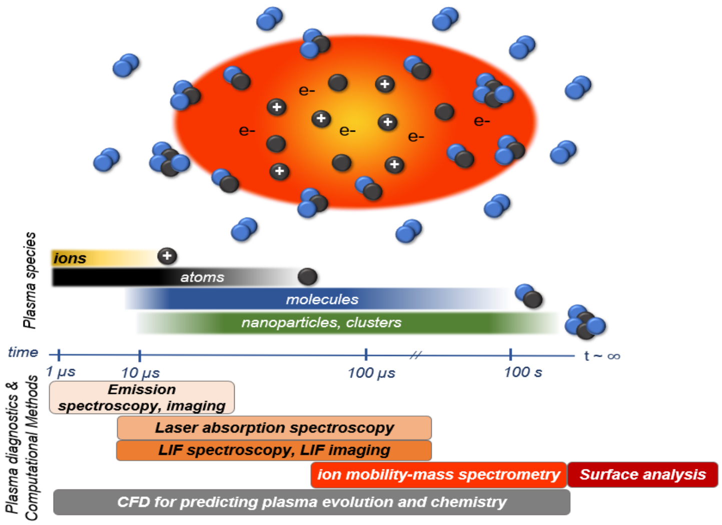

Figure 1: Illustration of plasma chemistry processes that evolve from atoms/diatoms to molecules, nanoparticle clusters formation within microseconds to longer timescale particulate formation and growth which are not understood well.

Approach: We developed and applied computational fluid dynamic (CFD) techniques to understand the intial stages of plasma formation and evolution of temperature and pressure fields after laser ablation.

Results

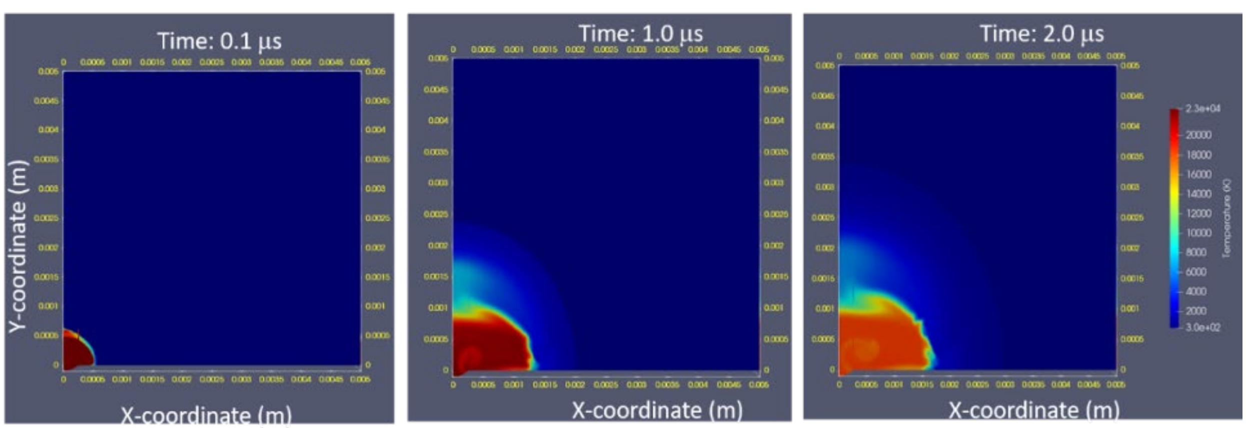

Figure 2: Snapshots of temperature (K) fields within Al plasma evolution during the first two microseconds simulated using the CFD OpenFOAM toolbox. The initial physical conditions are selected based on ns laser-produced plasma from an Al target. Modeling was performed in an inert Ar environment at 1 atmosphere.

An example of the time sequence of temperature evolution of laser-produced Al plasma in an inert environment is shown in Fig. 2. The selection of initial conditions was based on previous experimental results. The CFD simulation clearly shows that the plasma physical properties attain favorable conditions for plume chemistry within a short time after plasma onset. However, the plasma simulation involving plume chemistry is very complicated. CFD simulations can be extended to predict the kinetics of thermo and plasma chemistry by including the plasma-chemical reaction routes and by considering various reversible reactions with respective temperature-dependent rate coefficients. This work developed a modeling framework using CFD that will be used to investigate multi-component plasma chemistry conditions and ultimately connect to nucleation and particulate formation as the plasma cools down.

Impacts

This work brought together atmospheric scientists (M. Shrivastava) and NSD scientists (S. Harilal) to address a complex multidisciplinary problem that could benefit by application of integrated-modeling measurement techniques. A proposal using aspect of this work was submitted to DOE Office of Science fusion energy this year by S. Harilal. Additional proposals based on this work will likely be submitted in the near future, thus potential generating multi-disciplinary collaborations and funding.

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