PHYSICS BASED MODELING FOR NUCLEAR ROCKET FUEL DEVELOPMENT. R. Litchford,[1] W. Luo,[2] and J. Cassibry,[2] [1]NASA Marshall Space Flight Center (ron.litchford@nasa.gov), [2]University of Alabama Huntsville, Propulsion Research Center.

Introduction: Modern engineering development efforts for high-temperature nuclear rocket fuels are placing increased emphasis on early stage R&D using surrogates and/or depleted uranium along with artificial heating techniques to evaluate physico-chemical characteristics and optimize fabrication methods [1,2]. This approach is motivated by a desire to minimize costs and mitigate safety/security concerns as much as possible while obtaining critical engineering data leading to nuclear environment testing and fuels certification.

Alternative high-temperature fuel forms currently under consideration include graphite composites, CERMETs, and bi/tri-carbides. Potential processing techniques include HIP, traditional and advanced pressing/sintering, and consolidation of CVD coated powders. Much of this current effort is strongly focused on fabrication and testing of preliminary samples and prototypical fuel forms. Experience indicates, however, that unexpected and anomalous test results will likely occur and that meaningful progress will require a sound theoretical/modeling basis for interpreting, understanding, and resolving developmental issues. This is particularly emparative when utilizing non-nuclear evaluation methods where the energy deposition process does not exactly replicate fission energy release processes and considerable care must be taken in terms of designing experiments and interpreting test results.

To meet this need, we have undertaken the establishment of a comprehensive multi-physics modeling methodology incorporating fluid/solid mechanics, heat transfer, and computational electromagnetics. The fundamental approach relies on a large-scale continuum representation using a multi-material (i.e., solid, liquid, gas, plasma) smooth particle hydrodynamics (SPH) solver, which may be locally coupled with atomistic molecular dynamics (MD) to address multi-scale phenomena. Because of the importance of electromagnetic based energy deposition in non-nuclear testing methods, a finite-difference time-domain computational electromagnetics (FDTD-CEM) solver has also been incorporated.

The proposed implementation strategy is unconventional and innovative in that it relies on a gridless Lagrangian SPH method to evolve the continuum field while the electromagnetic field is advanced on a fixed background grid using an FDTD-CEM solver for the Maxwell equations. Because the SPH method is gridless, it may accomodate large elastoplastic distortions and model material damage from crack growth to fracture. In addition, the intrinsic multi-fluid capability permits the direct modeling of melt, moving multi-fluid interfaces, and free-surface deformable boundaries. To make the method more amenable for modern usage, the entire suite of solvers has been implemented as MATLAB code in order to leverage intrinsic structures for vector/matrix operations with the long term aim of exploiting parallel algorithmic procedures and the multi-threaded shared memory capability of multi-core graphics processing units (GPU). Moreover, MATLAB is a powerful high-level programming language that is portable, accessible, intuitive, and popular with modern science/engineering graduates.

Multi-Physics Modeling: A baseline 3D SPH code using the preceding system of equations has been implemented in MATLAB using a Störmer-Verlet leap frog algorith. This technique was selected because of its low memory requirements, efficiency, and exact time reversibility characteristics. The continmechanics uum conservation equations are evolved by this method using a time stepping constraint evaluated as the minimum of a CFL condition and a particle acceleration limit. Additional state-of-art numerical considerations incorporated into the computer code include artificial dissipation to minimize nonphysical oscillations and enable accurate shockwave capture; artificial heat to avoid excess heating effects when the flow is stagnated; and adaptive smoothing length to maintain accuracy and minimize numerical shot noise.

Efforts to validate the resulting SPH code include simulation of standard test problems from computational physics for which baseline analytical solutions are known. These include established shocktubes, viscous shear flow, and gas dynamic expansion problems in multi-dimensions and some basic solid mechanics problems. Test results thus far have been very good and continued validation and verification efforts are ongoing.

Computational Electromagnetics: Our basis for evolving the Maxwell electromagnetic field equations is an FDTD-CEM solver on a fixed Cartesian background grid. This approach is relatively simple to formulate and adapt for computer simulations and can be structured to accommodate massively parallel coding techniques. Moreover, it can easily handle arbitrarily shaped composite geometries consisting of different types of substances and materials.

Construction of the FDTD formulation proceeds via a discretization of the Maxwell curl equations wherein the divergence relations are intrinsically satisfied. Thus, each vector equation yields 3 coordinate components yielding a total of 6 FDTD updating equations for the electric and magnetic fields.

The Cartesian background grid on which the FDTD formulation is constructed is based on the well-known rectangular Yee cell convention whereby the electric field components are centered and aligned with the cell edges and the magnetic field components are centered and orthogonal to the cell faces. This special field component arrangement, therefore forms an interlinked array defining Faraday's law and Ampere's law contours. Material properties are distributed over the grid in association with the respective field component locations.

Thus, an FDTD-CEM solution proceeds by building a background Yee grid and assigning media property distributions to construct material objects and fluid distributions. The discrete staircase gridding does impose some restrictions on the geometrical accuracy by which a problem space can be represented, although local subcell modeling approaches can be implemented for improved fine structure resolution. For initial developmental purposes, however, a basic staircase FDTD model can provide sufficient accuracy and is deemed adequate.

Because of the desire to make the basic FDTD-CEM solver broadly useful and applicable to practical engineering applications and laboratory experiment configurations, coding modules should also be incorporated to account for the inclusion of lumped circuit elements. These include models for voltage/current sources, resistors, capacitors, inductors, and diodes as well as the ability to accommodate lumped element components distributed over a surface or volume.

A baseline 3D FDTD-CEM code has been implemented in MATLAB on the basis of the preceding developmental approach. The system of discretized updating equations for the EM fields are advanced in a leap frog time stepping fashion whereby the electric field components are evaluated at integer time steps and the magnetic field components are evaluated at half-integer time steps. These field values are then available to update Lorentz force and Joule dissipation effects. During the time marching procedure, the lumped circuit elements and material distributions may be updated, and data samples may be extracted to update real time plots. Numerical stability is maintained by imposing a CFL constraint on the maximum allowable time step. The resulting FDTD-CEM code has undergone extensive testing and validation studies with excellent results.

Results : Numerical model development and validation studies are ongoing with an emphasis on the establishment of baseline capability for typical fuel element test configurations of interest. Fig. 1, for instance, illustrates a solid model for a cylindrical fuel element sample with single coolant passage being heated by an rf-induction coil. The goal is to generate detailed multi-physics simulations to provide strong science based insight and guidance in support of advanced nuclear rocket fuel development.

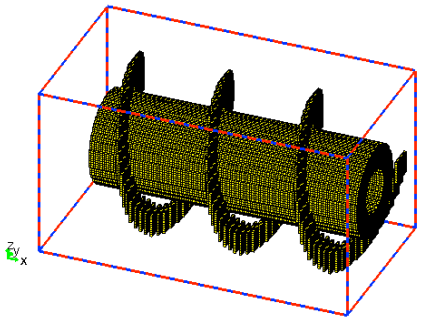

Fig. 1. Illustration of typical fuel element test configuration with rf-induction coil.

References:

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