Simulated Spectral and Imaging Diagnostics for Plasma Jet Experiments

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Presented at the LANL Plasma Jet Workshop
Los Alamos, NM, Jan. 24-25, 2008
Prism Research and Software Development Activities

• Prism is a scientific research and software development company located in Madison, WI (founded in 1998).

• Prism employs 5 Ph.D. physicists, with ~ 70 yrs experience in studying radiating plasmas.

• Research activities are focused on the study of HEDP plasmas. This work has been supported by:
  • DOE laboratories (Sandia, LANL, LLE)
  • government agencies (DOE, DOD, NSF, NASA).

• Our efforts are concentrated in the areas of:
  • plasma radiation physics
  • hydrodynamics and radiation transport
  • atomic processes and kinetics of non-LTE* plasmas
  • spectroscopy and atomic physics
  • scientific software development.

• Our work often involves the simulation and analysis of laboratory plasma measurements.
  => We write simulation codes, but work closely with experimentalists in the analysis of data (spectral, imaging).

* LTE = Local thermodynamic equilibrium.
Overview of Prism Simulation Tools

- Prism has developed a suite of codes applicable to studying plasmas spanning a wide range of conditions:
  - **HELIOS**: A 1-D radiation-hydrodynamics code (w/ MHD for cyl. geometry)
  - **HELIOS-CR**: HELIOS with inline non-LTE atomic kinetics
  - **SPECT3D**: A code for computing spectra and images – based on multi-D plasma distributions – that can be compared with experimental measurements
  - **PrismSPECT**: A “single-cell” spectral analysis package
  - **VISRAD**: A 3-D radiation analysis/CAD program for designing and modeling experiments at OMEGA, NIF, Z
  - **PROPACEOS**: Equation of state and opacity code
  - **PEGASYS**: Experimental spectral analysis package

- In developing these codes, we have put a substantial emphasis on making them easy to use, both for setting up simulations and viewing results. These codes are well-suited for:
  - government and commercial laboratory research and development
  - graduate and undergraduate student research and education

- These codes are currently being used at:
  - Major gov’t research laboratories (Sandia, LANL, LLE, AFRL, RAL, CEA, AWE)
  - Corporations & Research Organizations (Cymer, Siemens, Fox Chase Cancer Center)
PRISM Code Suite for Simulating Plasma Physics Experiments:
*HELIOS, SPECT3D, VISRAD, PrismSPECT, ATBASE, PROPACEOS, PEGASYS*

**VISRAD**
3-D View Factor and Target Setup Code

**HELIOS-CR**
1-D Rad-Hydro Code (inline C-R*)

**SPECT3D** Imaging and Spectral Analysis Package

**PrismSPECT**
Spectral Analysis Code

**Atomic Database**
- C-R* Atomic Data: ATBASE
- EOS: SESAME, PROPACEOS
- Opacities: PROPACEOS

**PEGASYS**
Experimental Data Graphical Analysis System

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*Laser parameters (λ_L, P_L(t))*

Incident Flux (ν, t) Throughout 3-D Surface Element Grid

**Plasma Distribution**
\[ T(r,t), \rho(r,t) \]

**Spectra, Streaked Spectra**
Images (Filtered, Monochromatic)
XRD signals
Instrumental effects

**Experimental Spectrum**

For grid of \( T, \rho, F_{ext} \), elements:
- Spectra
- Ionization fractions
- Atomic level populations

* C-R = Non-LTE Collisional-Radiative Modeling

**Best Fit** \( T, N_e \)
Overview

Prism support for HyperV plasma jet project includes:

• Modeling and data support for the LSP PIC code:*
  • Prism has developed 2-D flux-limited radiation diffusion algorithms that are now incorporated into LSP.
  • Prism has provided algorithms to support the use of PROPACEOS opacity and equation-of-state data in LSP.
  • New algorithms have been provided for LSP/P4 to generate NetCDF-formatted output files that can be read into SPECT3D.

• To support the direct comparison of PIC and MHD simulation results with experimental measurements, we have upgraded the SPECT3D package to:
  • Post-process the LSP output to generate simulated images and spectra.
  • Post-process output of MACH2 simulations.

• Spectral analysis calculations performed with PrismSPECT.

The primary goal of SPECT3D is to compute images and spectra based on simulation code output (e.g., rad-hydro, PIC) that can be directly compared with experimental measurements.

This provides a critical link in assessing the reliability/validity of simulation codes.

SPECT3D computes the radiation emission and absorption along a set of rays passing through the plasma.

A broad range of atomic processes for the plasma are computed in detail.
SPECT3D Imaging and Spectral Analysis Package

- SPECT3D is a collisional-radiative spectral analysis package used to compute:
  - Detailed emission and absorption spectra
  - Filtered images (e.g., x-ray framing camera, monochromatic images)
  - XRD signals

- A wide variety of 1-D, 2-D, and 3-D geometries are supported:
  - 1-D planar, cylindrical and spherical
  - 2-D Cartesian X-Y, cylindrical R-Z, spherical R-θ
  - 3-D Cartesian X-Y-Z (parallel domain-decomposition)

- Atomic level populations (LTE or Non-LTE), spectra, and images are computed for:
  - Plasma distributions from radiation-hydrodynamics or PIC simulation codes (LSP, MACH2, ALEGRA, CTH, DRACO, HELIOS, HYDRA, ...)
  - User-defined plasma distributions (1-D or 2-D) generated by PlasmaGen

- Time-dependent kinetics based on time-dependent hydro properties is supported.

- Radiative emission, absorption, & transport is computed for a grid of rays through a plasma.

- Radiographs can be computed using either continuum or line backlighters.

- SPECT3D is a user-friendly code that provides:
  - Direct comparisons between simulation results and experiment (images, spectra)
  - Tools for obtaining physical insight into the plasma radiative properties and experimental measurements.
Rad-Hydro & PIC Simulation Results Are Post-Processed with SPECT3D to Generate a Variety of Spectra and Images

- Emission spectra
- Streaked spectrum
- Monochromatic images
- Backlit images

$t = 0.6$ ns  $t = 1.0$ ns  $t = 1.4$ ns  $t = 1.8$ ns
Physics Modeling in SPECT3D and PrismSPECT

- Includes atomic processes for:
  - collisional ionization, recombination, excitation, deexcitation
  - spontaneous emission
  - radiative recombination, dielectronic recombination, autoionization
  - photoionization and photoexcitation

- Includes modeling for energetic particles (relevant to fast ignitor experiments):
  - non-Maxwellian electron distributions
  - relativistic electron cross sections
  - proton-impact excitation and ionization

- Line shapes include effects of natural, Doppler, Stark, and Auger broadening.

- The use of detailed atomic modeling is supported, including:
  - Satellite line emission/absorption, forbidden/intercombination transitions
  - Inner-shell bound-bound and bound-free transitions

- Computes effects of external radiation fields on atomic level populations & spectra.

- Includes effects of instrumental broadening on spectral and imaging results.
The ATBASE suite of atomic physics codes is used to generate high-quality atomic data for simulating plasma radiative properties over a wide range of conditions.

It utilizes several atomic structure and modeling codes, including Hartree-Fock, Dirac-Fock, configuration interaction, and distorted wave codes.

ATBASE generates a comprehensive set of atomic data for all ions of any atomic element.

ATBASE calculated data is supplemented by NIST data for available atomic levels/transitions.

=> “Hybrid” dataset with goal of being both “comprehensive” and “accurate”

Models include:

- Atomic energy levels and oscillator strengths
  - Computed using Hartree-Fock, Dirac-Fock and configuration interaction (CI) models. When available, experimentally-based energy levels and radiative data are utilized.

- Photoionization cross-sections
  - Cross-sections from Hartree-Fock calculations are utilized for both valence-shell and inner-shell transitions. Radiative recombination rate coefficients are calculated from the photoionization cross-sections.

- Electron collisional excitation and ionization cross-sections
  - Distorted-wave (DW) calculations are performed to generate cross-sections and rate coefficients.

- Autoionization rates
  - Configuration interaction (CI) calculations are performed to generate autoionization rates.

- Dielectronic recombination (DR) rate coefficients
  - For DR related to K- and L-shell spectra, electron capture rates are computed using autoionization rates and the detailed balance relationship. For lower ionization stages, total DR rate coefficients are based on semi-empirical models.
PROPACEOS Equation of State (EOS) and Opacity Data

- EOS data \([E(\rho, T), P(\rho, T), Z(\rho, T)]\) are computed for LTE and non-LTE plasmas (including mixtures) using a hybrid EOS model:
  - QEOS-type model in strong coupling regime (high \(\rho\), low \(T\))
  - “Isolated atom” model in weak coupling regime

- Single-group and multi-group opacities computed using complex atomic models and cross section data based on high-quality atomic structure codes.

- Both EOS and opacities have been compared with publicly available calculations & data.
• Left: PROPACEOS results showing sensitivity of Titanium opacity to temperature.
• Right: Comparison of PROPACEOS opacities for CH with TOPS (LANL) at two T’s.

Simulations of Fe absorption show good agreement with experiments performed at Sandia. Absorption spectroscopy measurements provide stringent tests for calculated opacities.
Simulations Using PROPACEOS and SESAME EOS Data Give Similar Results

- We have performed HELIOS radiation-hydrodynamics simulations using SESAME and PROPACEOS EOS data for radiation-driven shocks in CH, Al, and Au.

  => Results are very similar.

**Advantages of PROPACEOS**

- Provides data for materials/mixtures not in SESAME library.
- Computes tables for both LTE and non-LTE plasmas.
Post-Processing of MACH2 Output

- Output of MACH2 simulations were post-processed with SPECT3D.
- Images and spectra were computed for every 0.2 μs form 4 to 8.6 μs.
- Detectors positioned to observe radiation in axial and radial directions.
- “Optically thin NLTE kinetics” was used for CH₂ plasma.
- Images were computed for photon wavelength from 300 to 1200 nm.
Time History of Plasma Temperature, Density and Emission (MACH2)

Plasma density, kg/m³

Plasma Temperature, eV

Simulated images (axial)

4 µs  5 µs  6 µs  7 µs  8 µs
Simulated Time-Resolved Spectra Based on MACH2 Simulation

Axial direction

Radial direction

4 μs

6 μs

8 μs
Example of Space-Integrated Spectrum Based on LSP Simulation

Spectra are computed for non-LTE CH$_2$ plasma at $t = 1$ $\mu$s
Analysis of HyperV Plasma Jet Experimental Data

- Left: Shot 20070509-17, Hα and C II spectral lines
- Right: Shot 20070509-22, C II and C IV spectral lines

Preliminary analysis of time- and space-integrated spectral data observed in radial and axial directions indicate ion density of about $10^{16} \text{ cm}^{-3}$.

Plasma composition is H:C=3:1.

The calculations were performed with PrismSPECT with NLTE kinetics. (Radiation-dependent rates and instrumental broadening not included.)
Summary

• Post-processing of radiation-hydrodynamics and PIC code results using detailed atomic modeling can provide stringent tests for assessing the reliability of simulation codes used to study plasma jet experiments.

• Prism has provided support for LSP radiation modeling:
  • 2-D multi-group radiation diffusion modeling
  • Use of multi-group opacity and EOS tabular data
  • Ability to post-process LSP output with SPECT3D

• In addition to LSP, we have developed the capability to generate images and spectra based on MACH2 output using SPECT3D.

• Our goals in the future are to:
  • Apply SPECT3D to simulate spectra and images based on LSP and MACH2 output, and benchmark results against experimental data.
  • Further develop and benchmark radiation physics models in LSP, including 3-D radiation diffusion modeling.
  • Perform analysis of time-resolved spectroscopic data from plasma jet experiments.