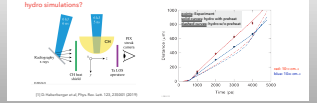
Species Separation and Hydrogen Streaming: The Physics of CH Shock Release Revealed by Molecular Dynamics Simulations

S. Zhang[1,*], S. X. Hu[1], D. Haberberger[1] A. Shvydky[1], V. N. Goncharov[1], and D. E. Fratanduono[2]
[1]Laboratory for Laser Energetics, University of Rochester, [2]Lawrence Livermore National Laboratory
*Email: szha@ile.rochester.edu

*This material is based upon work supported by the Department of Energy National Nuclear Security Administration under Award Number DE-NA0003856.

Shock release poses grand challenges to hydro simulations

- Recent experiments show low-density plasmas generated by shock released CH moving far ahead of what regular hydro (i.e., w/o radiation preheat) predicts
- Agreement is reached when considering **radiation transport** in hydro simulations, which induces expansion at the rear surface of CH before shock arrival
- Q: Is there any other microscopic physics that may have been missed in the single-fluid hydro simulations?



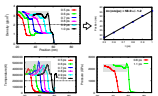
[1] D. Haberberger et al. Phys. Rev. Lett. 125, 215001 (2019)

We calculate the Hugoniot EOS to set a benchmark for the simulations

- Shock front position vs time ⇨ Shock velocity $U_s = d/\Delta t$
- Kinetic + virial contribution ⇨ Pressure $P = \rho_0 U_s u + \sum_{i=1,2,3} \frac{m_i \rho_0 u^2}{12} \frac{\langle r^2 \rangle}{\sigma^2}$
- Kinetic + ionization/energy partition ⇨ Temperature $T_e = \frac{P}{(1+Z)\rho}$, $P = \sum_{i=1,2,3} \frac{m_i \rho_0 u^2}{12}$

N_{ion}=50×50 mm cell with 1.55×10⁶ atoms; total kinetic energy: 1.05 g/cm³ ×(0.5 ps)² = 0.263 eV

[2] Kim Cheng et al., J. Chem. Phys. 142, 024910 (2015)



	U_s (km/s)	ρ (g/cc)	P (GPa)	T_e ($\times 10^4$ K)
DFT	52.5	3.8	2096	1.49
CMD	58.0 ± 1.2	3.0 ± 0.42	2022 ± 222	1.54 ± 0.36

* According to a DFT-based average-atom model for ionization [3], $\langle Z \rangle = 1.45$ at this temperature and density.
[3] S. X. Hu et al., Phys. Plasmas 23, 042704 (2016)

Hugoniot EOS from CMD agrees with DFT-MD to within 3%–20%

- Results are similar from calculations of samples with different density, structure, shock direction, and sizes and simulations with different time steps
- Results are overall similar when using AIREBO or REBO2 potentials

	U_s (km/s)	u_p (km/s)	P (Mbar)	ρ/ρ_0
ρ_0=0.9 g/cm³				
DFT	52	3.8	1.89	3.06
CMD	51.1 ± 0.9	3.8 ± 0.03	1.84 ± 0.04	3.03 ± 0.06
ρ_0=1.0 g/cm³				
DFT	54	3.9	2.40	3.51
CMD	53.1 ± 0.9	3.9 ± 0.03	2.34 ± 0.05	3.45 ± 0.06
DFT	56.5	4.1	3.15	3.85
CMD	55.4 ± 0.9	4.1 ± 0.04	3.09 ± 0.06	3.79 ± 0.07
DFT	59.5	4.4	4.19	4.19
CMD	58.4 ± 0.9	4.4 ± 0.04	4.11 ± 0.07	4.13 ± 0.07
ρ_0=1.2 g/cm³				
DFT	62	4.7	5.49	4.51
CMD	61.0 ± 1.1	4.6 ± 0.04	5.38 ± 0.08	4.51 ± 0.08
DFT	65.5	5.0	6.91	4.76
CMD	64.4 ± 1.1	5.0 ± 0.04	6.78 ± 0.09	4.76 ± 0.08
DFT	69.5	5.3	8.56	4.95
CMD	68.4 ± 1.1	5.3 ± 0.04	8.41 ± 0.10	4.95 ± 0.08
CMD, AIREBO*	68.4 ± 1.1	5.3 ± 0.04	8.41 ± 0.10	4.95 ± 0.08
CMD, REBO2*	68.4 ± 1.1	5.3 ± 0.04	8.41 ± 0.10	4.95 ± 0.08

Overall differences (relative to DFT-MD):
- ~10% in shock velocity
- 1%–20% in density
- ~40% in temperature
- 3%–12% in pressure

* Amorphous polystyrene (PS): 1.41 million atoms
* Syndiotactic (Syn): PS: 1.47 million atoms; Hexa: 1.-hexa: 1.-hexa: 1.-