Improvement of Capsule Mode 1 through Experimentally-Enhanced Monte Carlo Modeling

Target Fabrication Specialists Meeting

Sean Hayes
Sal Baxamusa, Juergen Biener, Tom Parham, Tom Braun, Xavier Lepro, Jean-Baptiste Forien, Liam Sohngen, Tobias Fehrenbach,Christoph Wild
LDRD 24-ERD-048

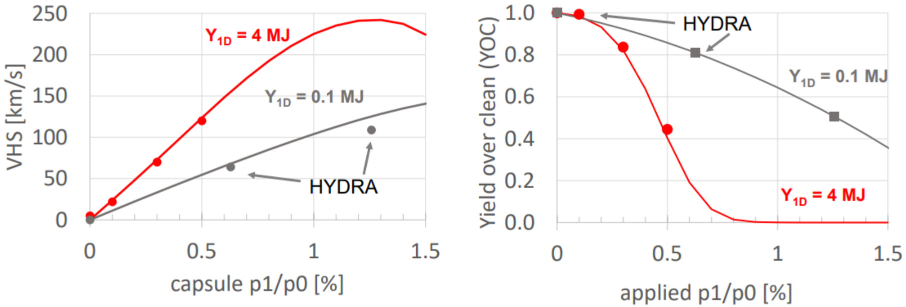
LLNL-PRES-867227
This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344. Lawrence Livermore National Security, LLC

Lawrence Livermore National Laboratory

What is P1 and how is it related to fusion yield?

- P1 develops during the coating process and is a wall thickness non-uniformity with a wavelength equal to the capsule circumference

- Per Hurricane et. al, ρR nonuniformities lead to asymmetric drives and residual kinetic energy of the hotspot



D. Casey

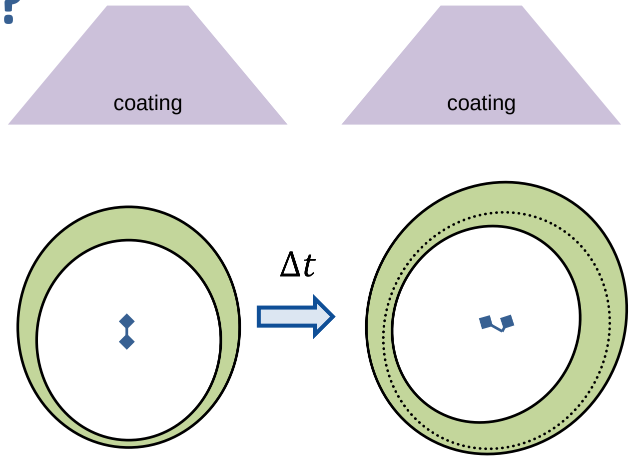
We only want to field the capsules with the lowest P1 on NIF, but other features (pits, inclusions) can narrow the batch yield significantly

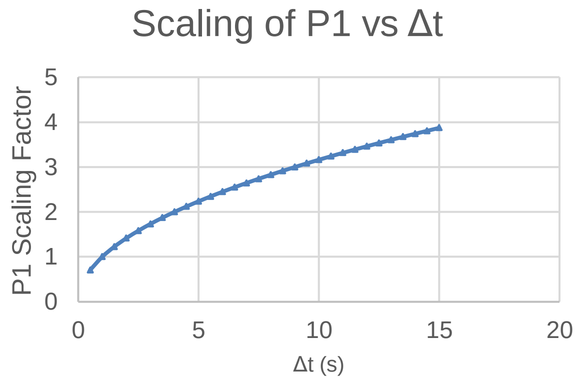
How does P1 arise in the coating process?

- During the CVD process, coating is added asymmetrically to the mandrel
- Reorientation to a random axis adds another Δd in a random direction
    - Can be modeled as a random walk
    - $P_1 \propto \sqrt{D\Delta d}$

D = Thickness

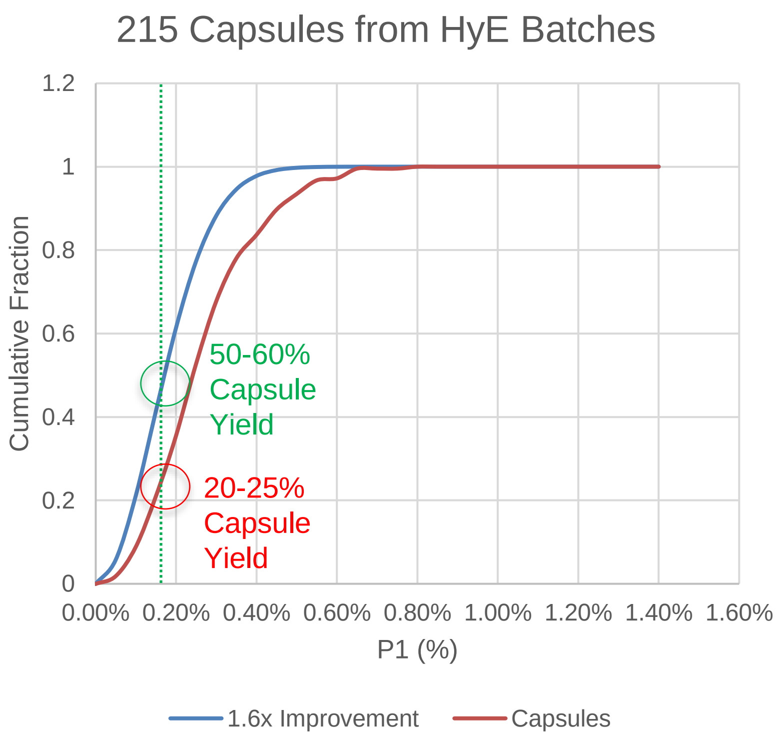
Δd = r x Δt





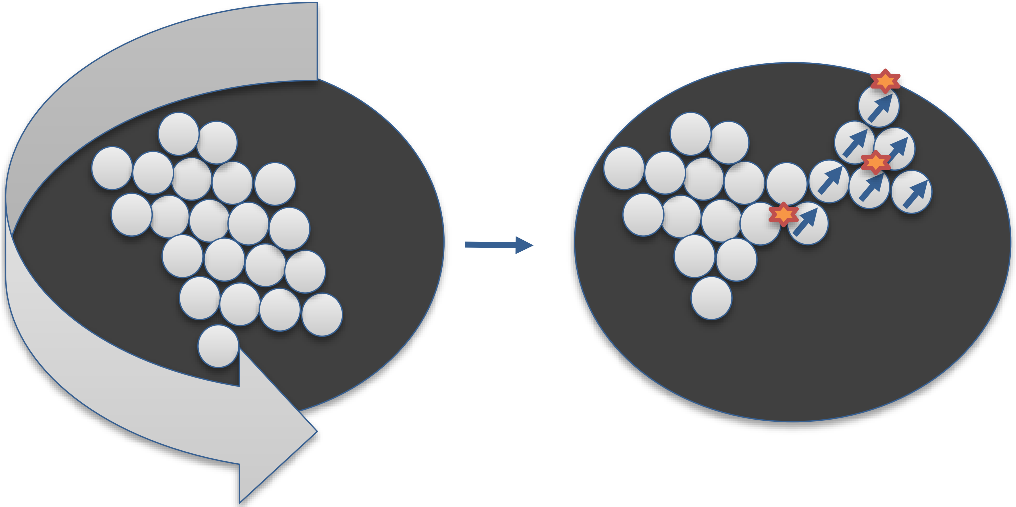
Modeling P1 as a 2D Vector with Uncorrelated Components Generates a Rayleigh Distribution

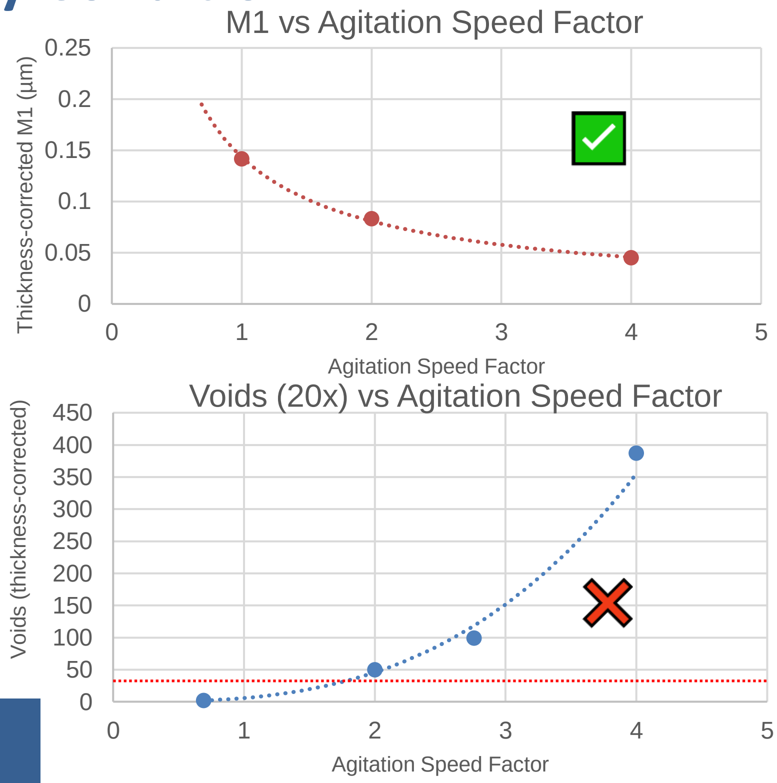
- The Rayleigh distribution is defined only by the significance factor σ
- Improving P1 by a factor of 1.6 would lead to a relative yield increase of more than **100%**
- **P1 is statistical – requires whole batch sampling**



Higher batch yields greatly enhances the number of experimental campaigns that can be supported – bespoke high-quality capsules are the primary bottleneck from a target fabrication perspective

The Simple Model Suggests Increasing Agitation Speed Will Reduce P1, but Voids form a Boundary Condition



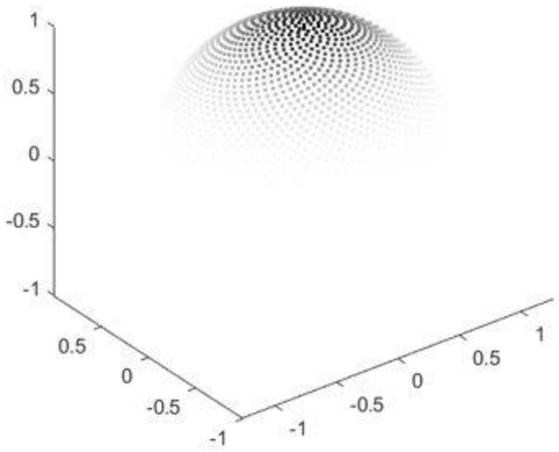


Exploring this parameter space is challenging, slow, and resource intensive

Monte Carlo Modeling Provides a Powerful Tool to Understand drivers of M1 and Optimization Pa

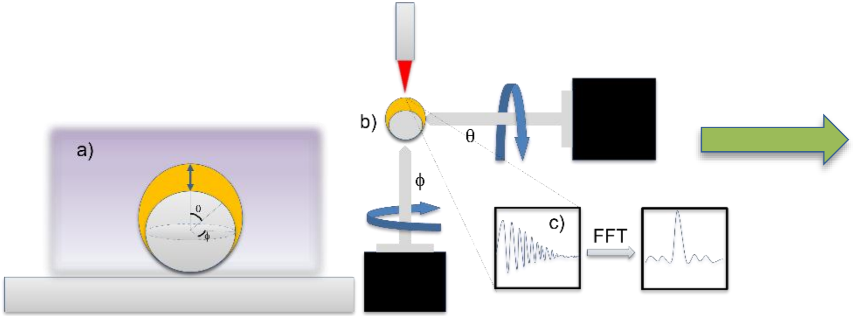
- Gathering basic data about HDC coatings in the current reactor can provide inputs for a simulated coater

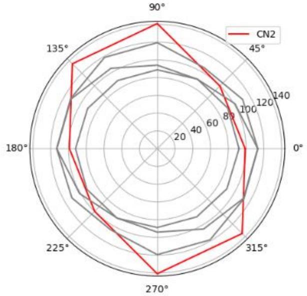
- Monte Carlo modeling is extremely fast relative to current experimental workflow (**coat > polish > Filmetrics/IR >Leach > CT**)

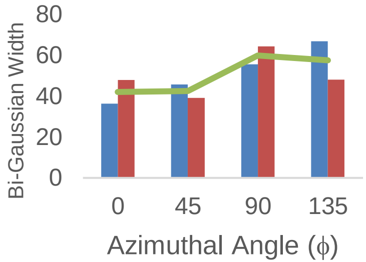


Simulation of a single coating event on an invisible spherical mandrel

The Key Inputs for MC Simulations are Basic Instantaneous Coating Non-Uniformity (ICNU) Data







Stationary shells are characterized by Filmetrics NIR measurements with control of both θ and ϕ

Characteristic ensembles (Coordination numbers) are analyzed to understand ICNU in a batch process

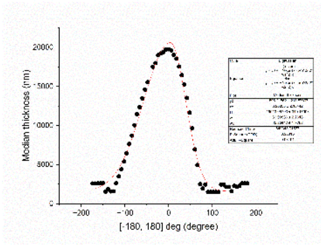
Knowing the ICNU for every coordination number and the distribution of coordination numbers allows for the Monte Carlo simulation of batch coatings

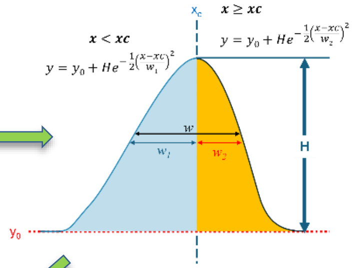
Bi-Gaussian Curve Fits to ICNU Generate One of Two Primary Inputs to Monte Carlo Simulations

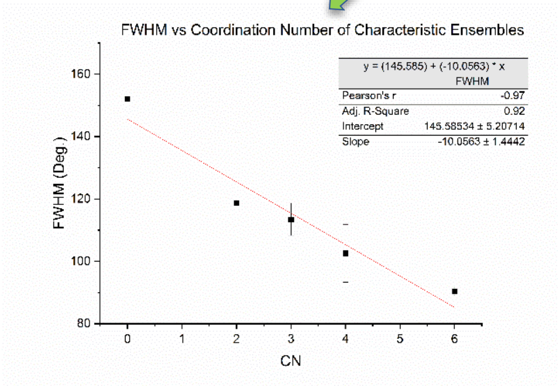
- Fitting the data to a bi-gaussian curve to extract the full width at half maximum (FWHM)
- Allows us to describe the shape of the HDC coating independent of thickness
- By setting a “rate” in the simulations and adjusting Δt the P1 can be tracked over time

Gaussian

$$y = y_0 + He^{-\frac{1}{2}\left(\frac{x-xc}{w}\right)^2}$$

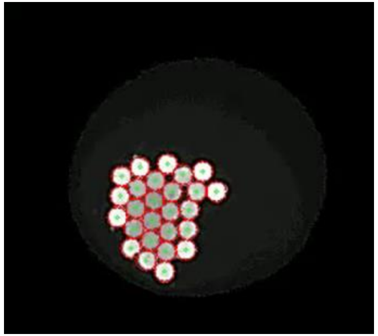


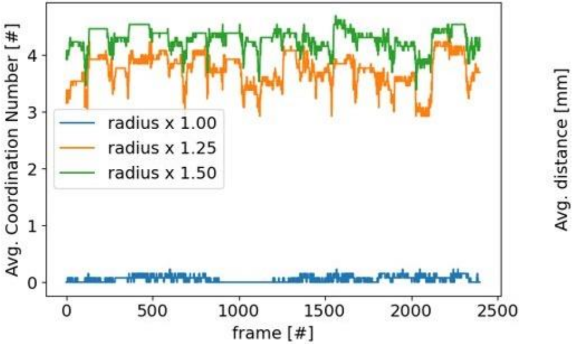




Motion Tracking Provides the Second Key Input

- The second input to the Monte Carlo simulation is the distribution of coordination numbers in a batch
- A novel method utilizing motion tracking and machine learning allows for the extraction of coordination number of each shell over every frame
- Distribution of coordination numbers provides the dice weighting for each mandrel in MC simulation

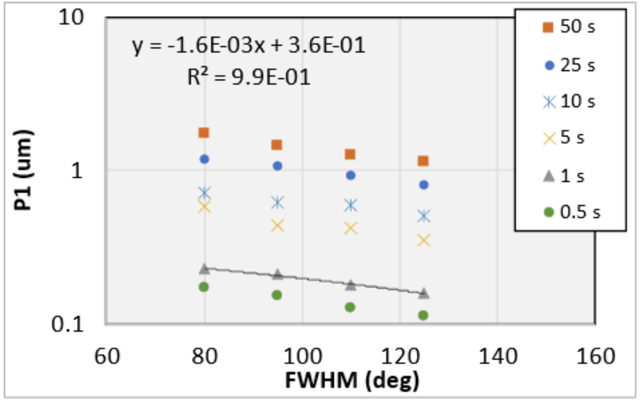


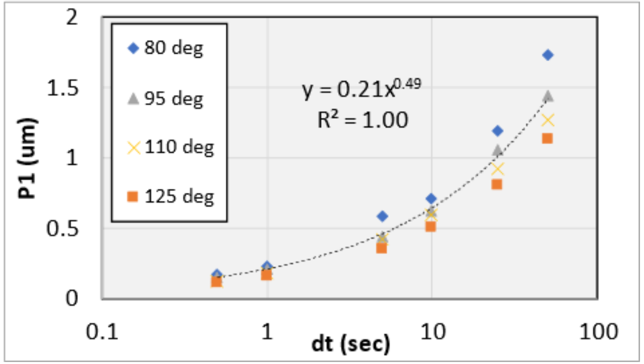


See poster from JB Forien for more details on this technique

Simulations show that M1 is sensitive to both Δt and Coating FWHM

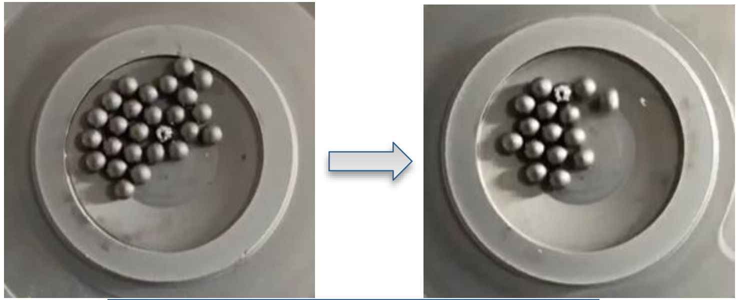
- Initial results from Monte Carlo simulations show that increasing the FWHM of the coating (decreasing the coordination number of shells) has a substantial M1 effect
- Studies on single shell vs batch processes have shown that voids are a result of shell/shell interaction rather than agitation speed
- Simulations of azimuthal asymmetry demonstrated that the only parameter that mattered was average FWHM, which is to be expected when Δt <<< the coating duration





Adjusting the FWHM to Study P1 Relationship

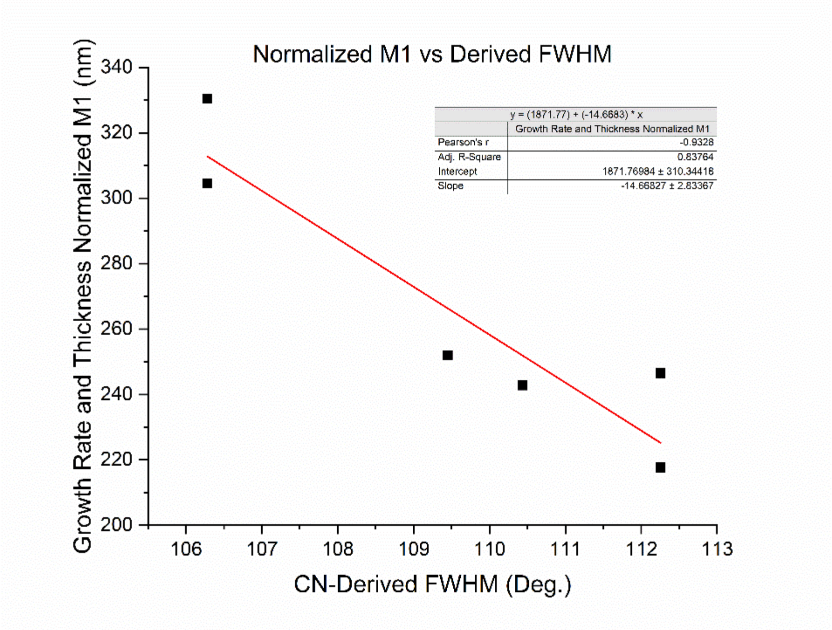
- Studying the relationship between P1 and FWHM is difficult, as we cannot tune FWHM *in-situ*
- FWHM can only be characterized by one set of coating parameters at a time – changing pressure, temperature, geometry, etc requires recalibration of ICNU



Reducing batch size reduces CN by reducing number of shells in the bulk

Simulations suggest that the FWHM effect is convoluted by changes in Δt

Batch Size	Prefactor C P1 = C $(dt)^{1/2}$	P1 (experiment, 85 um equiv)	dt
16	0.188	217.7	1.3
21	0.18	242.8	1.8
26	0.179	252	2.0
31	0.192	330.5	3.0
16 (redux)	0.182	217.7	1.4



Simulations allow us to estimate the relative contribution of FWHM and Δt on overall P1 –

Future Work

- Develop techniques to quantify the collision intensity of shells from motion tracking analysis
- Determine energy threshold for void generation
- Iterate on agitation schemes that minimize shell collisions and maximize shell randomization
- Cross reference with Monte Carlo Simulations to maximize impact of high cost experiments

Understanding the basic parameters and boundary conditions has the ability to reduce development time by orders of magnitude

Lawrence Livermore
National Laboratory