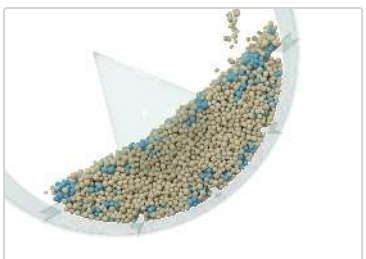
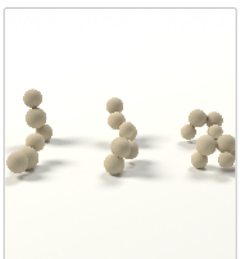
# TabletSimAI: from granulation to the coated tablet, one digital twin.

Not a single simulation. Multi-scale, multi-physics in one code: the whole process, from binder spray granulation to a coated tablet, each step handing its state to the next.



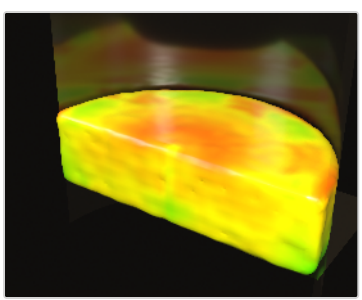
1. Granulation



2. Granule shapes



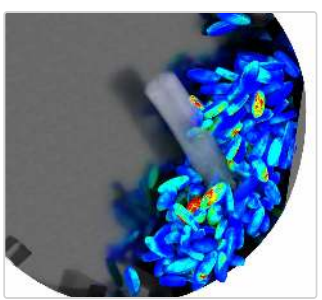
3. Mixer



4. Die compaction



5. Tablet



6. Coating

| Stage | Scale | Physics and handover |
|---|---|---|
| **1. Granulation** | **Molecular** | Molecular forces bind the granules.<br>Next: granules as clumps or polyhedra. |
| **2. Granule shapes** | **Granule** | Shapes extracted from the run, not sampled.<br>Next: into the blend. |
| **3. Mixer** | **Granules and fines, realistic size ratio** | DEM with cohesion laws.<br>Next: dose cut, DEM to SPH. |
| **4. Die compaction** | **Powder continuum** | Powder SPH holds density and stress.<br>Next: SPH to elements. |
| **5. Tablet** | **Solid** | Bonded polyhedral elements with the compact's stress and porosity.<br>Next: bonded tablet into later processes. |
| **6. Coating** | **Coated tablet** | Bonded tablet, SPH spray. |

**Scale progression: molecule to coated tablet.**

**Each material is calibrated once, never per simulation. After that the particle properties stay fixed, so a process change at any step can be followed through to the strength of the final tablet.**

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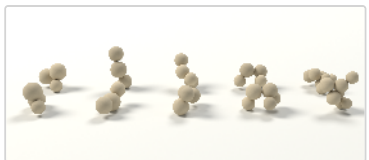
# The chain, from granulation to coating

The chain starts with the binder spray granulation. Tablet strength depends on how the blend fills the die, and each step hands its state to the next: the mass, lubricant and glidant are carried from the cut to the tablet.



**1. Granulation**
Binder spray forms the agglomerates.



**2. Granule shapes**
Agglomerates as clumps or polyhedra.



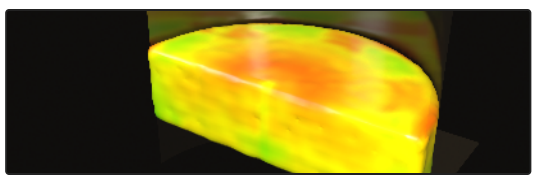
**3. Mixer blend**
Granules and fines at a realistic size ratio.



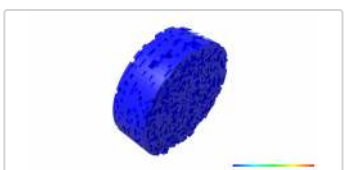
**4. Dose cut**
Cut from the blend, whole clumps kept.



**5. Die fill**
The dose settled in the die.



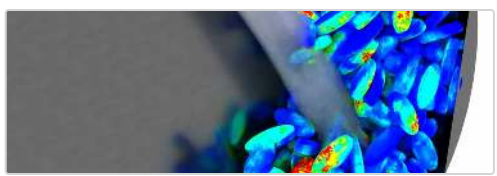
**6. Compaction**
Density and stress in the powder.



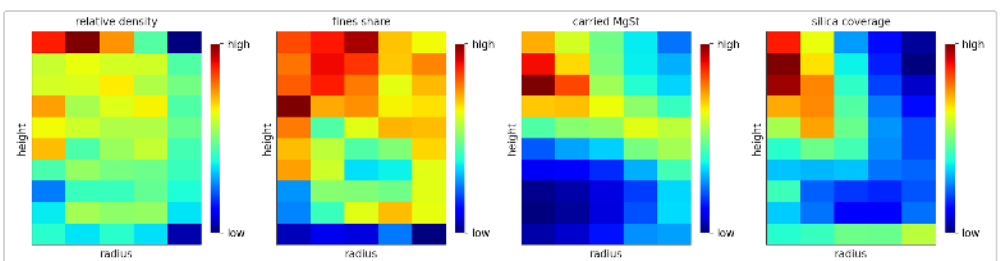
**7. Tablet**
Bonded solid with the compact's porosity.



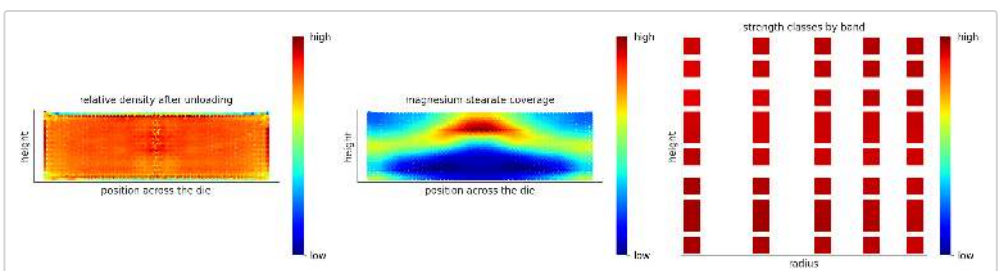
**8. Tests**
Strength test and ejection.



**9. Coating**
Caplet tablets under an SPH coating spray.




Die fill density, fines and excipient fields.

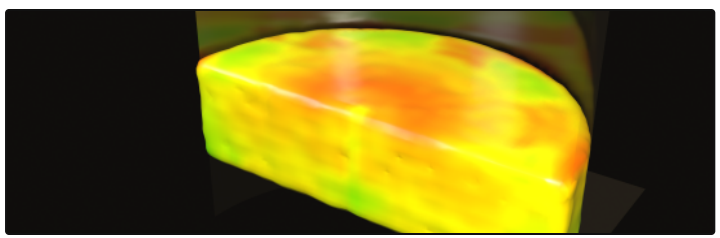



Compact density, lubricant coverage and strength classes.

# Die compaction, then the tablet

The powder is pressed as a continuum for the density and stress field in the die. The compact becomes a tablet of bonded solid elements that leaves the die intact and breaks in the strength test.

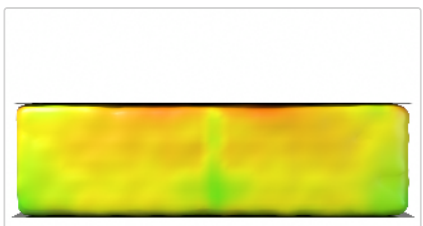
### Die compaction: stress in the powder, low (blue) to high (red), one scale



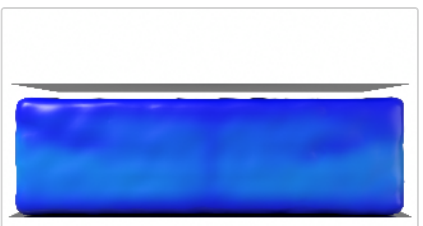
Cut open at peak load



Start

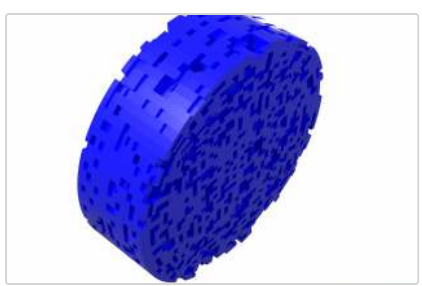


Peak load

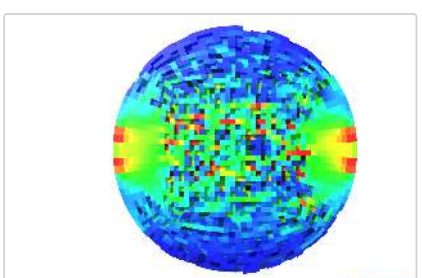


After unloading

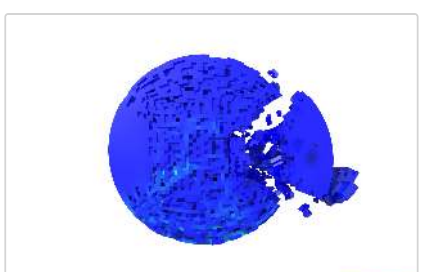
### The tablet: ejection, then the strength test



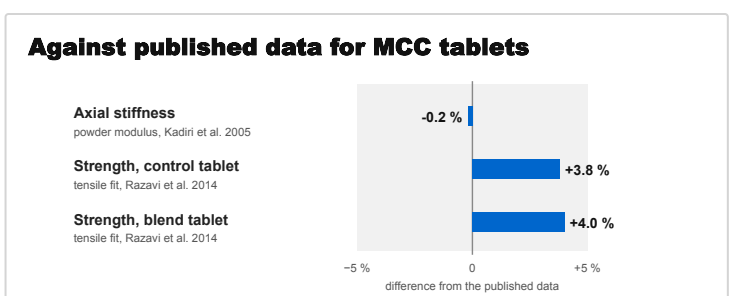
Ejected from the die, intact



Strength test, at the peak



After the split



# Coating: the tablet in a later process

A bonded tablet can be put into any later process and evaluated there. Here caplet shaped Element tablets tumble in a baffled drum under an SPH spray, and the coating collected on each tablet surface is tracked.

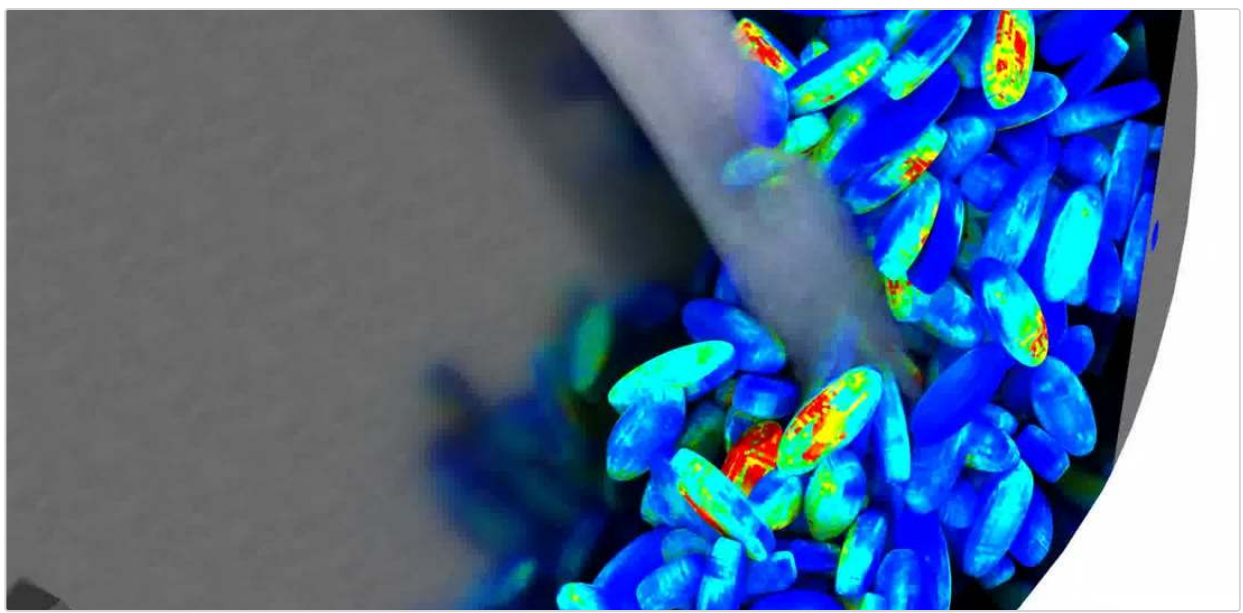
**Tablets coloured by the coating collected on each, low (blue) to high (red), one scale**



Spray start



Part way



Late in the run

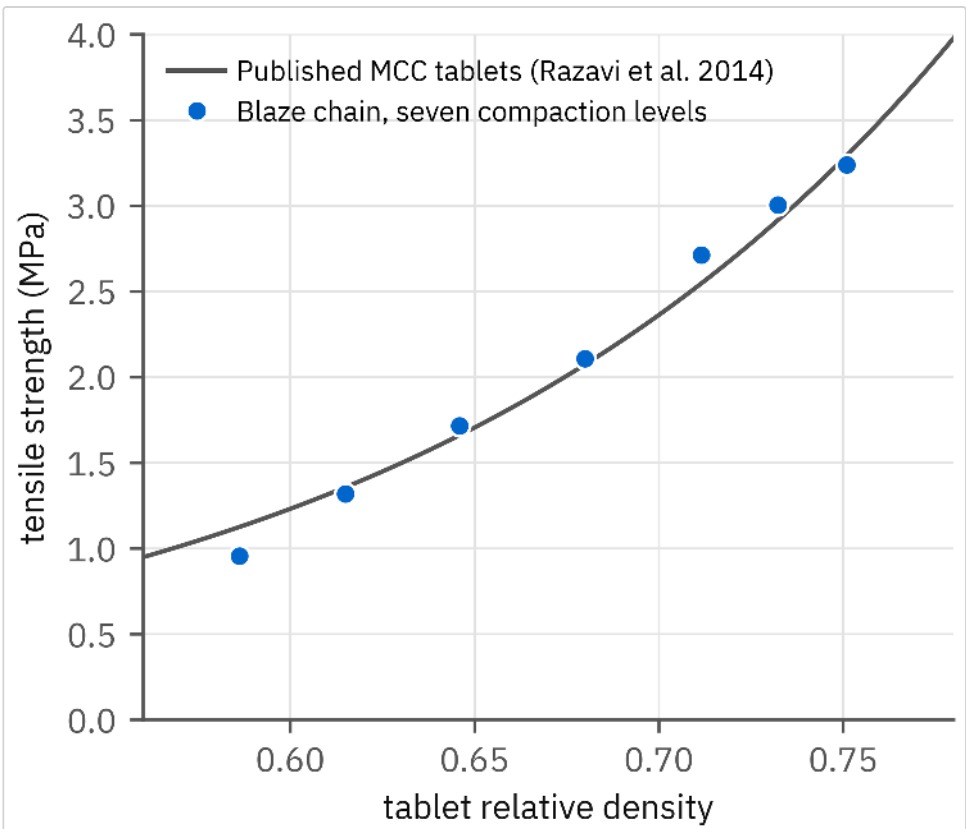
**The spread of coating between the tablets can be seen as they tumble through the spray. This run uses caplet shaped tablets, a different shape from the disc tablet of the chain.**

# TabletSimAI: a model that learns the whole chain

Because every step runs in one code with fixed material properties, the chain runs become training data. The model links a setting at any step to the strength of the final tablet.

| Stage | How the model learns |
|---|---|
| **1. Settings at every step** | Granulation: binder and drum. Mixer: time, lubricant, glidant. Die fill: dose and fill pattern. Compaction: punch force and speed. Coating: spray and drum speed. |
| **2. Blaze chain runs** | Granulation, mixer, die fill, compaction and tablet in one code, with the bonded tablet available for coating. Each run hands its state to the next step, so every run is a complete record from setting to tablet. |
| **3. TabletSimAI** | Trained on the chain runs. Predicts tablet strength with its uncertainty, and names the next runs that teach it most. |

**Ask what a process change does to the tablet before the press trial, from a model that knows the physics of every step.**




Tablet strength across seven compaction levels against MCC data.