IMAGE BASED MODELLING AND DIRECT NUMERICAL SIMULATIONS WITH GeoDict, THE DIGITAL MATERIAL LABORATORY

IBFEM-4i
Swansea, September 12th, 2019

Andreas Wiegmann
GeoDict® Module Overview

This is Innovation through Simulation

Math2Market GmbH
Selected Clients of a total of ~150 clients
**Typical Artifacts**

- Image Alignment
- Brightness
  - changes in cutting direction and in single images
  - Curtaining-effect / streaking, sensor dependent
  - Local charging leads to local change in brightness
- Non-invaded pores after resin infiltration
NANO-CT GRAY-VALUE CORRECTION

- Images can have changes in brightness
- Can be adjusted for each direction, x-, y-, and z-
- Can be beneficial in other use cases as well
  - Here: brightness correction of a nanoCT scan
Curtain Filter

Original SEM

SEM after applying the curtain filter
Applied Filters:
- Non-Local Means Filter
- Sharpen Filter
Identified grains using specialized watershed and subsequent grain reconnection.

- Removed grains at the domain boundary
STATISTICAL TWIN USING GRAINGEO

IMPORT GRAINFIND RESULTS INTO GRAINGEO

GeoDict

GeoDict

[Image of GeoDict software interface]

- Result File Name: GrainGeoCreate.gdr
- Create Options:
  - Create in Current Domain
  - Keep Current Objects / Structure
- Domain:
  - NX: 200 (200 μm)
  - NY: 200 (200 μm)
  - NZ: 200 (200 μm)
  - Voxel Length: 1 (μm)
- Generation and Overlap Mode:
  - Allow Object Overlap
  - Without (Remove) Object Overlap
  - Prohibit Object Overlap
  - Use Isolation Distance
  - Match Solid Volume Fraction Distribution
  - Enforce Object Overlap
- Stooping Criterion:
  - Fixed Object Number
  - Object Solid Volume Percentage (%): 35
  - Grammage (g/m²)
  - Density (g/cm³)
  - Object Weight Percentage (%)
  - Maximal Run Time (h): 6
- Random Seed: 45

OK Cancel
STATISTICAL TWIN USING GRAINGeo

- Used GrainGeo’s “Create Grains”
- Visual comparison is good
STATISTICAL TWIN USING GRAINGEO

COMPARISON OF STATISTICS

- Used GrainGeo’s “Create Grains”
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- However, statistics do not match perfectly
STATISTICAL TWIN USING GRAINGeo

COMPARISON OF STATISTICS

- Used GrainGeo’s “Create Grains”
- Visual comparison is good
- However, statistics do not match perfectly

Relative agreement of number of grains: 90%
Relative agreement of number of grain contacts: 154%
STATISTICAL TWIN USING GRAINGeo

GRAINGeo: ADD BINDER!

Slice from Grain Identification

Slice from
Used GrainGeo’s “Create Grains” and GrainGeo’s “Add Binder”
Visual comparison is good
COMPARISON CT-SCAN VS. DIGITAL TWIN

COMPARISON PLOTS

μCT-scan

2nd Digital Twin
COMPARISON CT-SCAN VS. DIGITAL TWIN

VISUAL COMPARISON

- Used GrainGeo’s “Create Grains” and GrainGeo’s “Add Binder”
- Visual comparison is good
- Statistics match nicely
COMPARISON CT-SCAN VS. DIGITAL TWIN

VISUAL COMPARISON

- Used GrainGeo’s “Create Grains” and GrainGeo's “Add Binder”
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- Statistics match nicely
DIGITAL BATTERY DEVELOPMENT

Solutions with GeoDict®

Dr. Ilona Glatt, Dr. Mathias Fingerle, Dr. Fabian Biebl, Sebastian Rief, Franziska Arnold, Steffen Schwichow, Dr. Barbara Planas
Li-Ion Battery

Challenges for Materials Design:
- Efficient Transport of Li-Ions
- Deposition of metallic lithium
- Mechanical Stress & Degradation
MICROSTRUCTURE OF A LI-ION – CATHODE

SCAN AND SEGMENTATION: BY COURTESY OF J. JOOS, KIT
MICROSTRUCTURE OF A LI-ION – CATHODE

SCAN AND SEGMENTATION: BY COURTESY OF J. JOOS, KIT
PARTICLE EXPANSION DUE TO LI-INTERCALATION
PARTICLE EXPANSION DUE TO LI-INTERCALATION
INFLUENCE OF ANODE GRAIN SIZE:

BATTERY DICT HALF-CELL SIMULATION

- Charging of an anode with different grain sizes
- Identical porosity, amount of connected active material and electrolyte
- At 2.5 C, charging gets harder with larger particles
Analysis of µCT scans of nonwoven samples

Andreas Grießler, Rolf Westerteiger, Steffen Schwichow, Andreas Wiegmann, Math2Market
Wesley DeBoever, Bruker µCT
Training Data: Use GeoDict’s unique fiber modelling capabilities:

- Modeled 10 Digital siblings (512x512x256 Voxels) as training data
- Varied fiber curvature, orientation, length and diameter
- Corresponded to ~1 billion solid voxels as training data points
Training Data: Then make the models look like binarized scans!

- All fibers in the models get the same gray value, just as in the segmented 3D scans.
TRAINING PHASE OF NN

Neural Network learns weights for edges

Dozens of Binarized GeoDict models

Dozens of Original GeoDict models
Usage Phase of NN

Segmented 3D scan

Neural Network with weights on edges

Labeled fibers for 3D scan
FIBER IDENTIFICATION BY NN: SUMMARY

Training: NN learns edge weights from input and output
- input: GeoDict Model: binarized version
- output: GeoDict Model: labeled fibers

Usage: NN predicts labeled output from input using weights
- input: Synchrotron / µCT data: binarized version
- output: Synchrotron / µCT data: labeled fibers
OVERVIEW OF SAMPLE STRUCTURES

- Carded nonwoven samples
- Scanned and stitched together by Bruker microCT
- Analyzed by Math2Market using GeoDict

<table>
<thead>
<tr>
<th>Sample Name</th>
<th>Resolution</th>
<th>Physical dimensions</th>
<th>Voxel dimensions</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>2.4µm</td>
<td>43.9 x 11.6 x 4.1 mm</td>
<td>18,310 x 4,816 x 1,704</td>
</tr>
<tr>
<td>B</td>
<td>2.7µm</td>
<td>42.2 x 10.9 x 4.8 mm</td>
<td>15,619 x 4,032 x 1,796</td>
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</table>
SAMPLE A – SEM VIEW

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SAMPLE B – SEM VIEW

Resolution   Physical dimensions   Voxel dimensions

2.7µm 42.2 x 10.9 x 4.8 mm³ 15,619 x 4,032 x 1,796
**FIBER ORIENTATIONS – SAMPLE A**

<table>
<thead>
<tr>
<th>XY</th>
<th>XZ</th>
<th>YZ</th>
</tr>
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<tbody>
<tr>
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View of a section of the surface in the direction of the X axis.
## Fiber Orientations – Sample B

View of a section of the surface in the direction of the X axis.

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<th>YZ</th>
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<tr>
<td><img src="image1" alt="Graphs" /></td>
<td><img src="image2" alt="Graphs" /></td>
<td><img src="image3" alt="Graphs" /></td>
</tr>
</tbody>
</table>
FiberFind was used on the complete sample. Process is explained on a smaller cutout.

The artificial intelligence separates the solid voxels in the image data into individual fibers. Each fiber becomes an independent, modifiable object which can be treated independently.

Geometric information, such as fiber length, fiber segment orientation and fiber diameter, can be read directly from the object.
DIGITAL PEM FUEL CELL DEVELOPMENT

Solutions with GeoDict®

Dr. Mathias Fingerle, Dr. Ilona Glatt, Dr. Jürgen Becker, Sebastian Rief, Andreas Grießer, Steffen Schwichow, Franziska Arnold
Challenges for Materials Design:
- Gas Permeability & Water Management
- Thermal & Electric Conductivity
- Operation at Elevated Temperatures (350 K)
- Mechanical Stress & Ageing
IMPORT OF A $\mu$CT SCAN WITH GeoDict®

DATA: $\mu$CT Scans of Toray TGP H 060, PSI Villingen (CH)

SEGMENTATION WITH ImportGeo-Vol
Data: \( \mu \text{CT} \) scans of Toray TGP H 060, PSI Villingen (CH)

1. Import
2. Analyze
3. Model
4. Design

Segmentation with Import GEO-Vol
The neural network in FiberFind-AI, can distinguished fiber and binder of a Toray Paper
The neural network in FiberFind-AI, can distinguished fiber and binder of a Toray Paper
CT-scan vs Digital Twin
Generated in GeoDict®

μCT-scan

Digital Twin
Conductivity in experiments did not fit conductivity in simulations.\(^1\)

- **Reason:** fibers and binder could not be differentiated.\(^1\)
- **Solution:** After identifying fiber and binder with *FiberFind-AI*, we can now run simulations where binder and fibers have different conductivity

GeoDict simulations with PoroDict & DiffuDict:

- Diffusivity and permeability calculated on Toray TGP H 060 at different compression level
- Comparison to experimental results in through plane (tp) and in plane (ip) direction
WATER SATURATION OF A GDL SIMULATED WITH SATUDICT
WATER SATURATION OF A GDL SIMULATED WITH SATUDICT

1. Analyze
2. Model
3. Design
MECHANICAL PROPERTIES: COMPRESSION OF GDL DETERMINED WITH ELASTODICT

- Transverse isotropic elastic modulus for fibers
- Isotropic elastic modulus for binder
- 30% compression
OPTIMIZE WATER MANAGEMENT WITH GeoDict® *

Motivated by Jens Eller, Paul Scherrer Institut
COMPRESSION OF POROUS MEDIA WITH GeoDict

μCT scans and alignment by Stefan Probst-Schendzielorz, Voith Paper, Heidenheim

VOITH
Compression of Generated Foams

Stress-strain curve calculated with GeoDict

Theoretical stress strain curve

- Foam generated with FoamGeo
- 80% compression (on deformed geometry)
- Buckling of cell walls can be observed
- Characteristical stress strain curve
- Constant positive pore pressure
Compression of Generated Foams

Theoretical stress strain curve

1. Linear elasticity,
2. Plateau
3. Densification

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Theoretical stress strain curve

I. Linear elasticity, 
II. Plateau 
III. Densification 

- Foam generated with FoamGeo 
- 80 % compression (on deformed geometry) 
- Buckling of cell walls can be observed 
- Characteristic stress strain curve 
- Constant positive pore pressure
COMPRESSION SIMULATION OF A DRAINAGE FELT

COMPRESSION @ 0.1 MPa

Scan
547 x 546 x 410 Voxel
0% Deformation

ElastoDict
547 x 546 x 410 Voxel
0% Deformation
COMPRESSION SIMULATION OF A DRAINAGE FELT

COMPRESSION @ 1.0 MPa

Scan
547 x 546 x 358 Voxel
-12.68% Deformation

ElastoDict
547 x 546 x 358 Voxel
-12.68% Deformation
Compression Simulation of a Drainage Felt
Compression @ 2.0 MPa

Scan
547 x 546 x 341 Voxel
-4.75% Deformation

ElastoDict
547 x 546 x 341 Voxel
-4.75% Deformation
COMPRESSION SIMULATION OF A DRAINAGE FELT

COMPRESSION @ 4.0 MPa

Scan
547 x 544 x 314 Voxel
-7.92% Deformation

ElastoDict
547 x 544 x 314 Voxel
-7.92% Deformation
COMPRESSION SIMULATION OF A DRAINAGE FELT

COMPRESSION @ 6.0 MPa

Scan

547 x 544 x 290 Voxel
-7.46% Deformation

ElastoDict

547 x 544 x 290 Voxel
-7.46% Deformation
SIMULATING EFFECTS OF PRINTING PROCESS IN ADDITIVE MANUFACTURING

Janna Krummenacker (IVW), Franz Schreiber (ITWM), Dr. Constantin Bauer (M2M), Andreas Grießer (M2M), Andreas Wiegmann PhD (M2M).

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CONTRIBUTIONS

This work requires 3D printing, 3D imaging, mechanical testing, CAD, simulation of the printing process and simulation of the mechanical properties.

- 3D printing by Math2Market GmbH, Kaiserslautern, Germany, using a commercial Ultimaker 3 printer
- Mechanical Testing by Institute for Composite Materials, IVW, Kaiserslautern
- 3D µCT imaging by Fraunhofer Institute for Industrial Mathematics, ITWM, Kaiserslautern
- CAD design of the meta material, simulation of the printing process and simulation of the mechanical properties by Math2Market GmbH, using GeoDict and Fraunhofer ITWM’s FeelMath
**WHAT IS SPECIAL ABOUT THIS MECHANICAL METAMATERIAL?**

In the **horizontal direction**, the material is rather stiff.

In the **other direction**, this material is initially very soft before turning into a very stiff material.
FUSED FILAMENT FABRICATION

SIMULATION ON DIGITAL MODEL

Meta-Material designed for Additive Manufacturing
Prototype manufactured by Additive Manufacturing
Problem: Standard approach to stiffness prediction is insufficient.
PROBLEM: STANDARD APPROACH TO STIFFNESS PREDICTION IS INSUFFICIENT

Simulated behavior does not agree with experiments
Simulation does not match experiment
Printing process is not modelled

- CAD Software / GeoDict modeling
- STL
- Print Parameters
- G-code
- 3D printer
- Physical part
- \( \sigma-\varepsilon \) curve

Printing Process
Simulation does not match experiment.
Printing process is not modelled.
SIMULATION DOESN’T MATCH EXPERIMENT BECAUSE PRINTING PROCESS IS NOT MODELLED

Questions

- Where does the discrepancy between the curves come from?
- Is it due to not modelling the printing process?
- Is it due to errors in the mechanics solver?
- Or even both?
### Validation of the Mechanics Solver

#### 1. µCT-scan and Import in GeoDict

<table>
<thead>
<tr>
<th>Printed Part</th>
<th>µCT-scanner</th>
<th>CT-data import</th>
<th>Segmented data</th>
</tr>
</thead>
<tbody>
<tr>
<td>in µCT-scanner</td>
<td>at Fraunhofer ITWM</td>
<td>into GeoDict</td>
<td></td>
</tr>
</tbody>
</table>
VALIDATION OF THE MECHANICS SOLVER

2. COMPARISON OF UNREALISTIC MODELED AND µCT SCANNED PART

unrealistic modeled part

µCT scanned part

Geometrical Validation
2. COMPARISON OF UNREALISTIC MODELED AND µCT SCANNED PART

Geometrical Validation
Overlap of Unrealistic modeled and CT scanned part

Geometrical Validation
Digital Image Correlation, Compression experiment

ElastoDict simulation on μCT-scan
Mechanics simulation agrees with experiment when applied to μCT scan.

Overlap of unrealistic modeled and CT scanned part.

Geometrical Validation

Property Validation

Overlap of Unrealistic modeled and CT scanned part.
PROBLEM WOULD BE SOLVED IF OUR MODEL WERE MORE SIMILAR TO THE µCT SCAN

CAD Software / GeoDict modeling

STL

Print Parameters

G-code

µCT scanned part

σ-ε curve

unrealistic modeled part

σ-ε curve

physical part

3D printer

Printing Process

© Math2Market GmbH
AND HERE, MAGIC HAPPENS...

INTRODUCING IMPORTGEO-AM

Take output of printer software and create 3D model that takes into account the printing process

unrealistic part
realistic virtually printed part
µCT scan of part

Geometrical Validation
SOLUTION: GEODict ENHANCED APPROACH TO STRESS-STRAIN PREDICTION MATCHES EXPERIMENT

The image shows a graph with the following legend:

- Red line: experiment
- Black line: μCT scanned part
- Green line: realistic virtually printed part
- Blue line: unrealistic modeled part

The graph plots stress in MPa against strain in %.

© Math2Market GmbH
Simulation of the printing process is necessary for correct prediction of the stress-strain curve.
Simulating the printing process leads to agreement of simulated and experimental curves.

1. **CAD Software / GeoDict modeling**
2. **STL**
   - Print Parameters
3. **Print**
   - G-code
   - 3D printer
4. **ImportGeo AM**
5. **Realistic virtually printed part**
6. **μCT scanned part**
7. **Physical part**
8. **σ-ε curve**

**Printing Process**
Modelling the printing process leads to agreement of stress-strain curves.

**Printing Process**

1. **STL**
2. **Print Parameters**
3. **G-code**
4. **3D printer**
5. **Realistic virtually printed part**
6. **σ-ε curve**

**CAD Software / GeoDict modeling**
CATALYTIC CONVERTERS, GPF AND DPF

Image source: https://www.thermofisher.com/blog/metals/new-reduced-platinum-catalyst-for-catalytic-converters/

Andreas Wiegmann, Anja Streit, Andreas Weber, Liping Cheng, Mehdi Azimian, Erik Glatt & Jürgen Becker
MODELING AFFTERTREATMENT USING RESIDENCE TIMES

Reactive flow simulation with AddiDict residence time tracking

For example in a car exhaust catalyst / DPF:
Reduction of Nox, HC and CO
Removal of soot
Flow simulation through channels and walls (porous catalyst).

Walls are modelled as porous material. Effective properties are computed from simulation on fully resolved scale.
Flow simulation through channels and walls (porous catalyst).

Walls are modelled as porous material. Effective properties are computed from simulation on fully resolved scale.
Simulate molecule motion in flow field and due to diffusion.

Bounces of the molecules at the interface between channel and the porous walls are available in GeoDict 2020.
Molecule Motion in Particulate Filter (plugged)

- Simulate molecule motion in flow field and due to diffusion.
- Bounces of the molecules at the interface between channel and the porous walls are available in GeoDict 2020.
SOOT DEPOSITION IN A HONEYCOMB
Flow simulation through channels, porous walls (dark gray) and reaction layer (blue). Used periodic boundary conditions to simulate much larger channel geometry. Use new feature of placing particles in specifiable locations (light gray area in the inlet).

\[ \text{CO, NO}_x, \text{HC} \rightarrow \text{CO}_2, \text{H}_2\text{O}, \text{N}_2 \]
Flow simulation through channels, porous walls (dark gray) and reaction layer (blue). Used periodic boundary conditions to simulate much larger channel geometry. Use new feature of placing particles in specifiable locations (light gray area in the inlet).
RESIDENCE TIMES IN CATALYST

- Track the residence times in channel, walls and reaction layer in GeoDict.
- Export the residence times for all molecules for postprocessing, for example for deriving reaction rates.

Total simulation time: 1s
Particles spend between 40% and 70% of the time in the wall. An around 7% of the time in the reaction layer.
**TWO SOURCES OF PRESSURE LOSS IN DPF**

1. Across the ceramic micro structure

2. Along the channels due to capillary forces

- We simulate them separately.

- In both cases, we simulate the loading of an initially clean filter.

---

567 µm
BINARIZED PMS IMAGES
FROM POLISHED MICROGRAPH SECTIONS AND
MODELED SINTERED CERAMICS
MEASURED POROSITIES & PERMEABILITIES
OF REAL CERAMICS VS MODELED POROSITIES & SIMULATED PERMEABILITIES ON MODELED CERAMICS

Simulation
Measurement
REDUCED PRESSURE DROP OVER TIME

After fast initial pressure drop increase (slope $s_1$, depth filtration phase) follows long slower pressure drop increase (slope $s_2$, cake filtration phase)
REDUCED PRESSURE DROP OVER TIME

After fast initial pressure drop increase (slope $s_1$, depth filtration phase) follows long slower pressure drop increase (slope $s_2$, cake filtration phase)
REDUCED PRESSURE DROP OVER TIME

After fast initial pressure drop increase (slope $s_1$, depth filtration phase) follows long slower pressure drop increase (slope $s_2$, cake filtration phase)

- Matched experiment with simulations
- Shortened depth phase to lower pressure drop during cake phase
- Fraunhofer IKTS manufactured ceramic, experiment matched simulations, and patent was granted: *Particulate filter, No. DE102012220181 A1*
At World Congress Experience 2018, Toyota Motor Company presented „Development of Low Pressure and High Performance GPF Catalyst“.
https://www.sae.org/publications/technical-papers/content/2018-01-1261/

GeoDict software helps to reduce back pressure in Gasoline Particulate Filters by 25%.

microstructure of wash coats analyzed, understood and improved with GeoDict
RENDERING OF MATERIALS AND SIMULATION RESULTS

Source: MANN+HUMMEL
GeoDict can also be used to export models for 3-D printing.

Source: MANN+HUMMEL on LinkedIn
Optimization of a virtual filter media prototype
Pushing the limits 2.0 – next generation

Source: MANN+HUMMEL
Simulation process automation with GeoPython
There is no free lunch – what did it take?

- Fiber characteristics
  - Fiber type
  - Fiber diameter \( d \)
  - Fiber shape \( a b^{-1} \)
  - Fiber orientation
- Fiber structure
  - Number of layers \( n \)
  - Fiber mix \( \varphi \)
  - Grammage \( G \)
  - Thickness \( t \)
  - Packing density \( 1-\varepsilon \)

Number of variations
- 1
- 5
- 4
- 3

Stochasticity \( \rightarrow \) multiple samples per design: \( 3 \times 60 \)
Total samples: 180

Size of one domain: \( 1024 \times 1024 \times 2048 \) voxels!
Computation time per simulation: \( \sim 2.5 \) weeks / \( \sim 420 \) hours
\( \Rightarrow \sim 75 \text{ k hours} \)

- manageable only by high degree of automation
- extensive use of GeoDict’s macro features

Source: MANN+HUMMEL
Simulation settings:
Domain: 512x512x768 voxel
Average velocity: 0.1 m/s
pH value: 3.2
Simulation time: 20 s
Number of particles: ~10,000
Runtime: 14 hs (16 cores)
CONCLUSION

- For fuel cells, batteries and aftertreatment catalysts, the material’s microstructure has a great influence on the performance
- The microstructure can be accessed by μCT, FIB-SEM & 3D image processing software
- The microstructure can be modelled by structure generators
- Material characterization can be done on images just as by experiments
  - Transport, Diffusion, Conduction
  - Stiffness, Deformation
- The development of next generation materials can be accelerated by screening designs digitally, first.
- You can do all this yourself with our easy-to-use, highly efficient and well-documented software
NEXT GENERATION MATERIALS WITH GeoDICT®

The materials of the future are within reach and we help you find them faster.

This is INNOVATION through SIMULATION