

Powerful Automation and Optimization Methods for Material and Process Analysis with Comsol Multiphysics and Matlab

BROAD BASE. BEST SOLUTIONS.

Dr. Thomas Frommelt Comsol Conference, Paris, 17th-19th November 2010

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Background

Matlab-based Automation

Controlling with Comsol Global Equations

Reverse Engineering of Transient Problems

Summary and Outlook



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SGL Group Best Solutions for our Customers



- High-performance graphite electrodes
- Carbon and graphite lining materials for blast furnaces



- Carbon and graphite cathodes in customized designs
- Fine-grain graphite for continuous casting





- High-purity fine-grain graphite for Si monocrystal-growing
- Coated graphite susceptors

Best in Class Products, Services and Ideas to satisfy current and future Needs of our Customers



SGL Group Best Solutions for our Customers



- Cylinder head gaskets
- Carbon ceramic brake discs
- Pump components made of carbon and graphite





- CFRP light weight components
- Fine-grain graphite for electrical discharge machining

High Temperature Technology



- Graphite heaters and insulation material
- C/C charging systems

Chemicals



- Sealing material
- Thermal decomposition units
- Multi-tube heat exchangers

Best in Class Products, Services and Ideas to satisfy current and future Needs of our Customers



SGL Group

- Leading manufacturer of carbon-based products with approx. 6.000 employees worldwide
- Centralized research and development: Technology & Innovation (T&I)
- Modeling group:
 - Material modeling
 - Product simulation
 - High-temperature processes
 - Heat and mass transport
 - Chemical conversion
 - High-temperature applications
 - Electro-thermo-mechanics
 - Induction heating



T&I Center





Electrode manufacturing

Brake discs



Graphite electrodes in arc furnace



Professional Background T. Frommelt

- Experimental Physics
 - PhD thesis on microfluidics at University of Augsburg in 2007
 - Acoustically driven flow (3, 4) in free-surface fluid circuits (1, 2)
 - Script-driven mixing optimization of highly laminar flow



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Metal Matrix Composite: Al–Infiltrated Graphite Task and Solution

- Target: Simulate material properties using the real microstructure
- Matlab image analysis:
 - Identify representative area
 - Segment into graphite, metal and voids
 - Transform into real or fitted microstructure
- Matlab-automated simulation
 - Rotate representative area
 - Setup microstructure
 - Thermo-mechanic application mode
 - Set properties of hundreds of subdomains
 - Generate periodic boundary conditions
 - Simulate thermal expansion





Metal Matrix Composite: Al–Infiltrated Graphite Results

 Excellent agreement of anisotropic coefficients of thermal expansion (CTE)

 Simulations of real microstructure and fitted microstructure yield comparable results





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Permeability Measurement Setup Analysis Task

- Permeability measurement by vacuum decay method
 - Slip flow of gas through porous material into an evacuated tank
 - Continuous pressure rise $p_{exp}(t)$ in tank
 - Experimental pressure change dp_{exp}/dt depends on material permeability



 Target: The model adjusts the material permeability k_{sim} such that model tank pressure p_{iv} follows experimental pressure p_{exp}(t)



Permeability Measurement Setup Analysis Solution



Permeability Measurement Setup Analysis Results

 Determines permeability including all effects like slippage or local sealing of specimen



Results of vacuum decay method agree with reference method

	Vacuum decay	Reference	
Specimen	method [mD]	method [mD]	Deviation []
1	2,75E+00	2,84E+00	-3%
2	3,17E+00	3,06E+00	4%
3	5,74E-01	6,01E-01	-4%
4	7,20E-01	7,35E-01	-2%
5	1,70E-01	1,66E-01	3%
6	1,11E-01	1,08E-01	2%





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Molding of Composite Sheets Task

- Molding of composite sheets
 - Fiber resin mixture in heated mold
 - Inhomogeneous curing is a relevant potential failure source:
 - Failure during further thermal processing
 - Bending of sheets





- Target: Develop temperature program for different sheet thicknesses
 - Homogeneous curing of resin
 - Minimum curing cycle time for high throughput



Molding of Composite Sheets Solution



Generate mold geometry

Create assemblies

Heat conduction application mode

Subdomain and boundary definitions based on constants

Interpolating functions with experimental results

Preliminary FEM structure

• 1st step: Reverse calibration of mold's thermal properties



Molding of Composite Sheets Solution



- Free optimizer fminsearch!
- 1st step: Reverse calibration of mold's thermal properties



Molding of Composite Sheets Solution



- 1st step: Reverse calibration of mold's thermal properties
- 2nd step accordingly: Reverse calibration of resin reaction model



Molding of Composite Sheets Results

Reverse simulation of thermal properties Determined mold 180 parameters fit Temperature Program 1 (°C) 08 001 heating experiments Exp. Temp. 1 Sim. Temp. 1 Exp. Temp. 2 Sim. Temp. 2 Exp. Temp. 3 Sim. Temp. 3 30 30 60 90 120 0 Time (min) Heating Rate 8.0 K/min Heating Rate 5.0 K/min Heating Rate 3.0 K/min Reaction model fits 0.7 0.7 0.7 80 0.6 0.6 0.6 **DSC** experiments 70 0.5 0.5 0.5 00 [7/8] 03 [7/8] Rate [W/g] Rate [W/g] DSC Heat Flow Rate [W/g] 0.4 0.4 Flow Flow 0.3 0.3 Reaction 0.3 40 DSC Heat DSC Heat 0.2 0.2 0.2 30 Total I 0.1 Ο. Ο. 20 Simulation Experiment Π 10 -0.1 -120 -0.1 -0. 0 └── 8K/min 140 160 120 160 120 140 160 180 180 140 180 5K/min 3K/min External Temperature [°C] External Temperature [°C] External Temperature [°C] Heating rates SGL GROUP **BROAD BASE, BEST SOLUTIONS.** 20 Dr. Thomas Frommelt – T&I Modeling THE CARBON COMPANY

Molding of Composite Sheets Results

- Unidirectional curing of thin sheets (peaks indicate reaction progress)
- Standard curing parameters lead to cured skin (top, bottom) and uncured core in thick sheets
- New curing parameters allow for unidirectional curing of thick sheets



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- Powerful techniques using basic features of Matlab and Comsol
 - Automation with Matlab
 - MMC microstructure generation
 - Mixing simulation



Permeability parameter search

- Optimization of transient tasks
 - · Heat transfer in mold
 - Reaction model





Permeability search







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Outlook More Tools

• Optimization with Comsol Optimization Module, e.g. optimized air curtain to screen factory building from chill through open gates



• Transient optimization with Comsol V4.x Optimization Lab



Outlook More Tools

• Analysis and optimization with OptiSLang:

