





BioDeg: corrosion/biodegradation simulation software for metallic biomaterials based on FreeFEM / PETSc / Qt

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BioDeg Software

- Multifunctional 3D simulation code for modeling biodegradation
- Cross-platform user interface
- Included pre- and post-processors
- FeeFEM/PETSc backend Qt frontend
- Available as an open source software

nulation Setup	8		Runn	ing		
Geometry & Mesh Materials & BCs Sol	ver Output		Stop sir	mulation		
Material properties		Computational problem size		Parallel computing info		
Material density (g/mm^3) Film density (g/mm^3)	0.001735	Degrees of Freedom (DOF) for each equation: Number of elements in the mesh:	110,119 640,249	Number of MPI processes: Average DOF in each MPI process:	6 23,451	
Saturation concentration (g/mm^3)	0.000134	Simulation progress				
Film porosity	0.55 🗘	Current step: 13 /	/81	Current time:	0.325/2	
Film tortuosity	1.00 ≑					16%
5		Volume reduction (mass loss): 3.22	2 %			
Reaction-diffusion properties						3%
Metal ion diffusion coefficient (mm^2/hour)	0.05000	Current task				
CI-ion diffusion coefficient (mm^2/hour)	0.05000	Task		Finished (last time) in		
OH- ion diffusion coefficient (mm^2/hour)	25.000	Solving interface tracking equation		1.92 seconds		
Film formation rate (1/hour)	7 ≑	Solving metal ion transport equation		13.45 seconds		
Film disolution rate (mm^6/hour.g^2)	10^ 10 🗢	Solving Cl- ion transport equation		11.79 seconds		
Convection properties		Solving film formation and elimination equal	1001	13.20 seconds		
Dynamic viscosity	0.850	Solving fluid flow equation				
Inlet velocity in X direction (mm/s)	0.10	Regulte visualization				
Inlet velocity in Y direction (mm/s)	0.00					
Inlet velocity in Z direction (mm/s)	0.00	Graphical output Metal ions concentration	View results	Plot mass loss	data	
Initial conditions		🛄 Mass los	is plot		×	
Initial CI- ion concentration (g/mm^3)	0.005175					
Initial pH	7.00 🗘			Mace loce ve time		
		2.76		ridda loda var unic	/	
tout						5
iput		2.07	/			
	/_//_1	1.38	1		-	
		0.69	/		-	
KU Leuven & Universit	v of Liege	0.00				
		i 0.0	JU 0.075	3 0.150 0.225 0	,300	

Statement of Need & Basic Concepts



Biodegradable Metals

- Mg, Zn, and Fe
- Gradually disappear/absorbed and replaced by new tissue/bone
- Great mechanical/biological properties
- The controlled release profile is an issue for different types of implants
- The degradation behavior should be tuned/optimized for various applications



(Han et al., Mater. Today, 23, 2019)

Problem Definition

- Challenge:
 - Tuning the biodegradation to the regeneration of the new tissue/bone
 - Optimizing the implant design based on the release profile
- Can be solved by:
 - Mathematical modeling of biodegradation
 - Coupling biodegradation models with tissue growth models
 - Considering environmental effects

Modeling Workflow



Chemistry of Biodegradation

The model captures:

- 1. The chemistry of dissolution of metallic implant
- 2. Formation of a protective film
- 3. Effect of ions in the medium
- 4. Change of pH



Mathematical Representation

Chemical reactions

$$Mg + 2H_2O \xrightarrow{k_1} Mg^{2+} + H_2 + 2OH^- \xrightarrow{k_1} Mg(OH)_2 + H_2$$
$$Mg(OH)_2 + 2Cl^- \xrightarrow{k_2} Mg^{2+} + 2Cl^- + 2OH^-$$

State variables

$$\begin{aligned} C_{Mg} &= C_{Mg}(\mathbf{x}, t) \quad C_{Film} = C_{Film}(\mathbf{x}, t) \\ C_{Cl} &= C_{Cl}(\mathbf{x}, t) \quad C_{OH} = C_{OH}(\mathbf{x}, t) \quad \mathbf{x} \in \Omega \subset \mathbb{R}^3 \end{aligned}$$

Derived Partial Differential Equations

$$\frac{\partial C_{Mg}}{\partial t} = \nabla \cdot \left(D_{Mg}^{e} \nabla C_{Mg} \right) - \nabla \cdot \left(\mathbf{v} C_{Mg} \right) - k_1 C_{Mg} \left(1 - \beta \frac{C_{Film}}{[Film]_{max}} \right) + k_2 C_{Film} C_{Cl}^2$$

$$\frac{\partial C_{Film}}{\partial t} = k_1 C_{Mg} \left(1 - \beta \frac{C_{Film}}{[Film]_{max}} \right) - k_2 C_{Film} C_{Cl}^2$$

$$\frac{\partial C_{Cl}}{\partial t} = \nabla \cdot \left(D_{Cl}^{e} \nabla C_{Cl} \right) - \nabla \cdot \left(\mathbf{v} C_{Cl} \right)$$

$$\frac{\partial C_{OH}}{\partial t} = \nabla \cdot \left(D_{OH}^{e} \nabla C_{OH} \right) - \nabla \cdot \left(\mathbf{v} C_{OH} \right) + k_2 C_{Film} C_{Cl}^2$$

Capturing the Moving Biodegradation Interface



Computational Model Implementation





Constructing Computational Model

- Discretizing PDE equations, numerical computation
 - Finite difference method (temporal derivatives)
 - Finite element method (spatial derivatives)
- Adaptively refined mesh generation (Euler mesh)





Implementing Computational Model

- Mesh generation (SALOME, Mmg), #Tetrahedra ~ 10M 20M
- Weak form implementation (FreeFEM), #DoF of each PDE ~ 2M 4M
- Parallelization is essential
 - High-performance domain decomposition (HPDDM)
 - High-performance preconditioners and solvers (PETSc)
- Paralleled IO postprocessing (ParaView)

Level Set Implementation

- Penalization for interface BCs
- Problem of concentration oscillation
- Computing $\nabla_n C_{Mg}$ correctly
- Problem of re-distancing the distance function ϕ

$$\nabla_n C = \frac{C(\mathbf{x} + h.n) - C(\mathbf{x} + 2h.n)}{h},$$
$$\mathbf{x} \in \Omega \subset \mathbb{R}^3$$



(Bajger et al., Biomech. Model., 2017)



Considering Convection

- Adding fluid flow and considering the effect of hydrodynamics condition
- Requires dealing with Navier-Stokes equations

$$\begin{cases} \rho \frac{\partial \mathbf{u}}{\partial t} + \rho(\mathbf{u} \cdot \nabla \mathbf{u}) - \mu \nabla^2 \mathbf{u} + \nabla p = 0\\ \nabla \cdot \mathbf{u} = 0 \end{cases}$$

- Implementing a parallel fluid flow code in FreeFEM (with fieldsplit preconditioner)
- Comparing the output of the CFD code with OpenFOAM (simpleFOAM)

https://github.com/mbarzegary/navier-stokes-solver

Parallelizing Computation

- Distributing the mesh among available resources
 - High-performance mesh decomposition
 - Overlapping Schwarz method
- Solving the linear system of equations
 - HYPRE BoomerAMG preconditioner
 - Fieldsplit preconditioner (for fluid flow)
 - GMRES iterative solver





Simulation and Parallelization Results





Orthopedics Screw Degradation



Porous Scaffold Degradation





Jaw Bone Plate Degradation





Narrow Cuboid



(Barzegari et al., Corrosion Science, 190, 2021)

Narrow Cuboid - pH Change



High diffusion (Saline solution)

Low diffusion (Buffered solution)

(Barzegari et al., Corrosion Science, 190, 2021)

Quantitative Results for Validation



(Barzegari et al., Corrosion Science, 190, 2021)

Comparing Fluid Results with OpenFOAM



The chamber with inlet and outlet, used to simulate hydrodynamics condition

Fluid velocity magnitude (top: in-house code, bottom: OpenFOAM)

Degradation with Flow





Parallel Strong Scaling Analysis (# of tetrahedra ~ 900K)



- Sequential part: 1%
- Parallel part: 99%



(Barzegari et al., Int. J. High. Perform. Comp., 35, 2021)

Preconditioner/Solver Performance



Solving level set PDE Solving Mg PDE Solving film PDE

(Barzegari et al., Int. J. High. Perform. Comp., 35, 2021)

Software Development





BioDeg: An Interface on FreeFEM Code

 Cross-platform, customizable, and adaptive UI developed using Qt and C++

aulation Setun	9				
nulation setup		Ru	nning		
Geometry & Mesh Materials & BCs Solver Output		Stop	simulation		
Fundamental equations	Computational problem size		Parallel computing info		
Solve metal ion transport equation	Degrees of Freedom (DOF) for each equation	n: 110,119	Number of MPI processes:	6	
Solve film formation and elimination equation	Number of elements in the mesh:	640,249	Average DOF in each MPI process:	23,451	
Solve CI- ion transport equation	Simulation progress				
Solve OH- ion transport equation	Current step:	12/81	Current time:	0.3/2	
Solve interface tracking equation					14%
Fluid flow equation	Volume reduction (mass loss):	2.76 %			
Solve fluid flow equation					2%
Solve full Navier-Stokes equation	Ourseast tank				
Write fluid velocity and pressure in VTK output	Taek		Einiched (lact time) in		
Solve fluid equation every 10 🗘 time steps	Solving interface tracking equation		1.81 seconds		
	Solving metal ion transport equation		13.11 seconds		
Time control	Solving CI- ion transport equation		12.33 seconds		
Time step (hour) 0.0250	✓ Solving film formation and elimination e	quation	1.43 seconds		
Final simulation time (hour) 2.00	Solving OH- ion transport equation		13.88 seconds		
Parallel computing	Solving fluid flow equation				
Enable parallel computing					
Number of narallel processes (CPLIMPT cores)					
number of parallel processes (CPO/MPI CORES) 6					
Redistancing control (advanced)					
Redistance the level set distance function					



Configuring the Simulation

Simulation Setup			
Geometry & Mesh	Materials & BCs	Solver	Output
Geometry & Mesh Materials & BCs Solver (Import external mesh Create mesh using Import mesh File Scaffold label Medium label Wall label (for fluid flow simulations) Inlet label (for fluid flow simulations) Outlet label (for fluid flow simulations) Outlet label (for fluid flow simulations) Create mesh Length of the container box (mm) Degrading cuboid size in X direction (mm) Degrading cuboid size in Z direction (mm) Degrading cuboid size in Z direction (mm) Mumber of nodes on the edge of the box Mesh refinement Refine initial mesh Refinement tolerance (error) Minimum element size	ng Tetgen		
Import mesh			
File			
Scaffold label			1 ‡
Medium label			2 🌲
Wall label (for flui	d flow simulations)		3 ‡
Inlet label (for flui	d flow simulations)		4 ‡
Outlet label (for fl	uid flow simulation	s)	5 ‡
Create mesh			
Length of the cont	tainer box (mm)	(20.00 ‡
Degrading cuboid	size in X direction (mm) (13.00 🗘
Degrading cuboid	size in Y direction (i	mm) (13.00 🗘
Degrading cuboid	size in Z direction (r	mm) (4.00 🤤
Number of nodes	on the edge of the l	box	32 🤤
Mesh refinement			
Refine initial m	esh		
Refinement tolera	ince (error)	(0.010 🤤
Minimum element	size	(0.040 🤤
Maximum element	t size	(0.800 ‡

(alticle) is a second backing (almost 2)	0.00000
nitial conditions	
Inlet velocity in Z direction (mm/s)	
Inlet velocity in Y direction (mm/s)	0.00
Inlet velocity in X direction (mm/s)	0.10
Dynamic viscosity	0.850
Convection properties	
Film disolution rate (mm^6/hour.g^2)	10^ 10
Film formation rate (1/hour)	7
OH- ion diffusion coefficient (mm^2/hour)	25.000
Cl- ion diffusion coefficient (mm^2/hour)	0.0500
Metal ion diffusion coefficient (mm^2/hou	r) 0.0500
eaction-diffusion properties	
Film tortuosity	1.00
Film porosity	0.55
Saturation concentration (g/mm^3)	0.00013
Film density (g/mm^3)	0.00234
Material density (g/mm^3)	0.00173
Aaterial properties	

imulation Setup	Simulation Setup
Geometry & Mesh Materials & BCs Solver Output	Geometry & M
Fundamental equations	Output option:
✓ Solve metal ion transport equation	🗌 Write VTK
✓ Solve film formation and elimination equation	Output direc
✓ Solve Cl- ion transport equation	Output name
✓ Solve OH- ion transport equation	Save results e
✓ Solve interface tracking equation	Save last s
Fluid flow equation	Text output
Solve fluid flow equation	Write the
Solve full Navier-Stokes equation	Multiply hydr
Write fluid velocity and pressure in VTK output	
Solve fluid equation every 10 🗘 time steps	Export degradi
Time control	Export sca
Time step (hour) 0.0250	Time betwee
Final simulation time (hour)	Export as
Parallel computing	Save initial me
✓ Enable parallel computing	Save initia
Number of parallel processes (CPU/MPI cores) 3	🗌 Save initia
Redistancing control (advanced)	
\checkmark Redistance the level set distance function	
Time between each redistancing (hour) 1.00	

Geometry & Mesh	Materials & BCs	Solver	Output
Output options			
🗌 Write VTK ou	tput		
Output director	y		—
Output name	output		
Save results even	rv	0.25	1 hour
Save last state	e of simulation		
lext output			
Write the evo	lved gas output per u	nit area	
Multiply hydroge	en evolution by		1.00
Export degrading	geometry		
Export scaffo	ld geometry during d	eoradatio	n
Time between e	ach export (hour)	-	1.00
Export as volu	ume mesh		
Export as sur	ace mesh		
Eave initial much (for dobugging)		
save micial mesh (ror debugging)		
		<i>c</i> .	
Save initial m	esh in a VTK file (afte	r refinem	enc)

BioDeg Preprocessor

- Developed using ParMmg and FreeFEM to embed a mesh into a container
- Mesh refinement on the corrosion interface

	reprocessor	mesn generator		
nput / output				
Part mesh				
Output file				
Generate VTK output as well for visualizati	on			
Container box		Mesh refinement		
Margin on each side along the X axis (mm)	5.00 ‡	✓ Refine mesh on the material-solution in	nterfa	ace
Margin on each side along the Y axis (mm)	5.00 ‡	Distance threshold for refinement	0.10)0 (
Margin on each side along the Z axis (mm)	5.00 \$	Refinement tolerance (error)	0.00	8
Number of nodes on the edge of the box	60 ‡	Minimum element size	0.10	00
Parallel computing		Maximum element size	3.00	00
Fnable parallel mesh generation		Mesh boundary approximation	1.00) (
Number of parallel processes (CPI I/MPI cores)	3	Mesh gradation value	1.30) (
remote of parameter processes (er offer cores,	, <u> </u>	Number of nodes on the edge of the box	3	4
Generate mesh		Stop process		

BioDeg Preprocessor



BioDeg Postporcessor

- Developed using Python and Qt Charts
- · Basic integration at this moment
- Will consider better integration options like ParaView Glance in the future

e View Tools Help		
nulation Setup	6 Running	
Geometry & Mesh Materials & BCs Solver Output	Stop simulation	
Material properties Material density (g/mm^3) D.001735 Film density (g/mm^3) D.002344	Computational problem size Parallel computing info Degrees of Freedom (DOP) for each equation: 110,119 Number of MPI processes: 6 Average DOF in each MPI process: 23,451	
Saturation concentration (g/mm^3) 0.000134 Film porosity 0.55 \$ Film tortuosity 1.00 \$	Smulation progress Current step: 13 / 81 Current time: 0.325 / 2	16%
Reaction-diffusion properties Metal ion diffusion coefficient (mm^2/hour) 0.05000	Volume reduction (mass loss): 3.22 %	3%
Cl-ion diffusion coefficient (mm^2/hour) 0.05000 OH-ion diffusion coefficient (mm^2/hour) 25.000 Film formation rate (1/hour) 7 ♀ Film disolution rate (mm^6/hour.g^2) 10 ♀	Task Finished (last time) in ✓ Solving interface tracking equation 1.92 seconds ✓ Solving metal ion transport equation 13.45 seconds ✓ Solving G-ion transport equation 11.79 seconds ✓ Solving in transport equation 11.79 seconds	
Convection properties Dynamic viscosity 0.850 Infet velocity in X direction (mm/s) 0.10 Infet velocity in X direction (mm/s) 0.00 Infet velocity in Z direction (mm/s) 0.00	✓ Solving OH-ion transport equation 13.20 seconds ✓ Solving fluid flow equation 13.20 seconds Results visualization Graphical output (Metal ions concentration ∨ View results) Plot mass loss data	
Initial conditions 0.005175 Initial CI-Ion concentration (g/mm^3) 0.005175 Initial pH 7.00 ©	Mass loss plot ×	
	2.07	8
KU Leuven & University of Liege +> Version: 0.8 <+	0,000 0.075 0.150 0.225 0.300	

Open Source and Open Science





Hosted on GitHub

- BioDeg core (FreeFEM, PETSc)
- BioDeg UI (Qt, C++)
- BioDeg pre-processor (FreeFEM)
- BioDeg docs



A Final Note ©

- A project to share experiences on scientific computing using open-source tools
- More info: TuxRiders.com YouTube.com/TuxRiders







Thank you for your attention



https://mbarzegary.github.io

MojBarz

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