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An Applied Nonlinear Approach to Predicting Enamel Demineralization and Remineralization Cycles

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Abstract
Enamel demineralization and remineralization are cyclical processes that influence the onset and progression of dental caries. This paper proposes a predictive framework based on nonlinear mathematical modeling to capture the complex interplay of biochemical, mechanical, and environmental factors that govern these processes. By integrating patient-specific variables such as salivary flow rate, biofilm composition, and local pH variations, the proposed model leverages bifurcation analysis and phase-portrait techniques to identify threshold conditions that demarcate the transition from a remineralizing equilibrium to one dominated by demineralization. Small perturbations in these parameters can generate substantial shifts in the system's behavior, at times resulting in rapid enamel loss or, conversely, enhanced mineral recovery under favorable circumstances. This approach offers a more robust representation of clinical outcomes than traditional linear models, as it accounts for feedback loops and nonlinear interactions often observed in vivo. In addition to elucidating the mechanisms behind caries progression, the model provides a scientific basis for personalized prophylactic strategies, allowing clinicians to predict and intervene at critical junctures. Combining high-resolution imaging data with real-time patient monitoring can further refine model parameters, increasing predictive accuracy and enabling clinicians to tailor treatment regimens more effectively. By analyzing how incremental shifts in salivary composition or microbial activity affect enamel mineral equilibrium, practitioners gain valuable insights into the interplay between host factors and environmental triggers of caries. These findings guide the development of interventions that promote enamel remineralization and suppress pathogenic bacterial colonization, ultimately improving long-term oral health and reducing the global burden of dental caries.
Keywords: *Demineralization, enamel, nonlinear modeling, remineralization, tooth decay*

INTRODUCTION

Enamel demineralization and remineralization are dynamic and opposing physiological processes that continuously occur in the oral environment. They are governed by a delicate balance between demineralizing forces, such as acidic metabolic byproducts from cariogenic bacteria and remineralizing agents, including calcium and phosphate ions supplied by saliva. This balance is modulated by multiple intrinsic and extrinsic factors such as dietary sugar intake, frequency of food consumption, fluoride exposure, oral hygiene practices, salivary flow and buffering capacity, microbial biofilm dynamics, and even genetic predisposition [1-3]. Traditional modeling techniques, often based on linear or simplified assumptions, provide useful insights into general trends but lack the sensitivity to accurately reflect the nonlinear and time-dependent nature of enamel mineral exchange. For example, linear models may fail to predict threshold effects, such as a sudden acceleration in demineralization when the pH falls below a critical level or the influence of dynamic feedback loops between plaque acid production and salivary buffering. These limitations highlight the need for more sophisticated modeling tools that can accommodate system instability, temporal delays, and emergent behavior.

To address this, our study introduces a nonlinear modeling framework rooted in the principles of dynamical systems theory. This approach allows the investigation of steady states (equilibria), system responses to perturbations, bifurcation points (where qualitative changes in behavior occur), and attractor dynamics (how the system tends to evolve over time). By mapping these features, it becomes possible to simulate and predict complex clinical phenomena, such as why certain individuals with similar diets and hygiene practices exhibit different caries risk profiles.

Moreover, this framework offers the potential to guide preventive strategies by identifying sensitive control parameters, such as improving saliva buffering or shifting oral microbiota that can steer the system toward a remineralizing regime. Such insights are invaluable for the development of precision oral healthcare and can support the implementation of personalized caries risk assessment and management protocols.

MATERIALS AND METHODS

1. Study Design and Participants

This study employed a prospective, observational design carried out over a six-month period at a university-affiliated dental clinic. The primary objective was to collect clinical and biochemical data relevant to the demineralization-remineralization cycle of tooth enamel and integrate them into a nonlinear mathematical framework. A total of 60 participants (male and female), aged between 18 and 45 years, were recruited through open-call announcements and dental checkups. Participants were stratified into three subgroups based on caries risk: low, moderate, and high, as determined by initial DMFT (Decayed, Missing, and Filled Teeth) scores and oral hygiene indices.

Inclusion criteria included:

- The presence of at least 20 natural teeth
- No history of active orthodontic treatment within the past year
- No current use of systemic antibiotics, corticosteroids, or antiseptic mouthwashes
- Willingness to follow all study protocols and attend follow-up appointments

Exclusion criteria included:

- Systemic illnesses that could affect salivary composition (e.g., diabetes, Sjögren's syndrome)
- Pregnancy or lactation
- Recent (<3 months) professional dental cleaning or fluoride therapy
- Use of medications known to alter saliva flow

2. Nonlinear Modeling Framework

2.1 Data Collection

Each participant underwent a baseline clinical examination, after which stimulated saliva was collected using paraffin wax chewing to assess:

- Salivary flow rate (mL/min)
- Buffering capacity, via titration with lactic acid
- Salivary pH, using a calibrated digital pH meter

Simultaneously, plaque biofilm samples were collected from the buccal surfaces of posterior teeth using sterile microbrushes. The following parameters were quantified:

- Colony-forming units (CFU) of Streptococcus mutans and Lactobacillus spp.
- Lactic acid production, via enzymatic assay
- Plaque pH drop curve, recorded over 30 minutes post-sucrose exposure

These variables served as input parameters for the mathematical model.

2.2 Model Formulation

To simulate enamel dynamics, we developed a system of coupled nonlinear differential equations. The model included the following key components:

- Mineral ion balance: tracking calcium and phosphate loss/gain
- Bacterial metabolic activity: modeled through nonlinear kinetics, incorporating substrate limitation and acid production
- Salivary buffering and ion diffusion: represented through time-varying source and sink functions

The governing equations included nonlinear feedback terms to account for autocatalytic acid generation, saturation kinetics in remineralization, and threshold responses to pH changes.

$$\frac{dM}{dt} = k_1 \cdot S(t) - k_2 \cdot B(t) \cdot f(pH(t))$$

Where M is mineral content, S(t) is salivary remineralization potential, B(t) is bacterial acidogenic activity, and f(pH) is a nonlinear pH-dependent factor.

2.3 Analytical Tools

The system of equations was solved using MATLAB with built-in Runge-Kutta solvers and symbolic computation tools for bifurcation analysis. Phase-plane portraits were constructed to visualize the dynamic behavior of the system under different parameter regimes. We performed bifurcation analysis to identify critical thresholds where minor shifts in biofilm acidity or salivary buffering would result in a qualitative change from remineralization to net demineralization.

In addition, sensitivity analysis was conducted to determine which variables had the greatest influence on system stability. This was done using partial derivative-based local sensitivity coefficients and global Monte

Carlo simulations.

3. Statistical Analysis

All experimental data were tabulated in SPSS v26 and analyzed using descriptive statistics (mean, standard deviation) and Pearson correlation coefficients to assess the relationships between salivary parameters and predicted mineral loss.

Model output was validated by comparing predicted changes in enamel mineral content to digital radiographic measurements (via standardized bitewing radiographs) using pixel intensity analysis and confirmed by cross-referencing with enamel surface microhardness data in a subset of participants.

Statistical significance was defined as $p < 0.05$ for all tests. Model accuracy and fit were assessed using root mean square error (RMSE) and R-squared values comparing predicted vs. observed mineral levels over time.

MATERIALS & METHODS

1. Study Design and Participants

This prospective, observational study was conducted over a period of six months at a university dental research center. The study was approved by the institutional ethics committee, and all participants provided informed consent.

A total of 60 systemically healthy volunteers, aged 18 to 45 years, were recruited. Participants were divided into three subgroups (n = 20 each) according to their individual caries risk status (low, moderate, and high), which was assessed using the DMFT index, oral hygiene score, and salivary pH.

Inclusion criteria included:

- At least 20 natural teeth present
- No fixed orthodontic appliances
- No antibiotic or steroid use within the last 3 months
- No history of systemic conditions affecting saliva or enamel health

Exclusion criteria:

- Xerostomia or salivary gland disorders
- Pregnancy or lactation
- Use of high-fluoride mouthwashes or remineralizing agents in the past 4 weeks
- Recent professional cleaning or restorative treatment

2. Data Collection

2.1 Saliva Analysis

Stimulated saliva was collected via paraffin wax chewing for 5 minutes, and the following parameters were recorded:

- Flow rate (mL/min)
- Resting pH and buffering capacity (via titration curve)
- Calcium and phosphate ion concentrations, using colorimetric assay kits

2.2 Plaque Analysis

Biofilm samples were obtained from the buccal surfaces of molars using sterile curettes. The samples were analyzed for:

- Acidogenic potential (measured via pH drop after sucrose challenge)
- Bacterial load, specifically S. mutans and Lactobacillus spp., using CFU counts and qPCR
- Enzyme activity, such as lactic acid dehydrogenase (LDH)

2.3 Enamel Hardness Testing

A subset of 15 participants (5 from each risk group) underwent enamel surface microhardness testing using a Vickers microhardness tester. Measurements were taken at baseline and after a 30-day observation period.

3. Nonlinear Mathematical Model

3.1 Model Structure

We developed a dynamical system consisting of three ordinary differential equations (ODEs), simulating:

- Mineral loss/gain in enamel ($M(t)$)
- Biofilm acid production ($B(t)$)

• Saliva buffering/ion diffusion (S(t))

Each equation incorporated nonlinear terms to represent enzymatic saturation, acid feedback, and threshold effects related to critical pH values (≈5.5).

$$\frac{dM}{dt} = k_1 S(t) - k_2 B(t) \cdot f(pH(t))$$

$$\frac{dB}{dt} = \alpha C(t) \cdot \left(1 - \frac{B(t)}{B_{max}}\right) - \beta B(t)$$

$$\frac{dS}{dt} = \gamma - \delta S(t) + \epsilon \cdot \cos(\omega t)$$

Where:

• M(t) = enamel mineral density
• B(t) = bacterial acid output
• S(t) = salivary buffering capacity
• Constants k_1, k_2, \alpha, \beta, \gamma, \delta, \epsilon, \omega were determined experimentally or estimated from literature [1–3]

3.2 Numerical Analysis

Equations were solved using Runge-Kutta 4th-order method in MATLAB.

• Bifurcation diagrams were plotted to identify thresholds for transition from remineralization to demineralization.
• Phase portraits were used to visualize long-term system behavior and equilibrium points.
• Parameter sensitivity analysis assessed which variables had the greatest effect on enamel outcome.

4. Model Validation and Statistical Analysis

• Predicted changes in enamel mineral content were compared to microhardness and digital radiograph data using RMSE and R^2 values.
• Descriptive statistics, Pearson correlation, and ANOVA were performed in SPSS v26.
• A p-value < 0.05 was considered statistically significant.

Figures & Tables

Key variables and parameters used in the nonlinear differential equations modeling enamel demineralization and remineralization cycles. The table includes dynamic system components (mineral content, bacterial activity, salivary response), biochemical influences (substrate concentration, pH) [4], and kinetic constants representing physiological rates and environmental oscillations. Units are provided for consistency in computational modeling.

Table 1. Model Variables and Descriptions.

Variable	Variables and Descriptions	
	Description	Units
M(t)	Enamel mineral content over time	mg/cm
B(t)	Bacterial acid production level	Mol/L
S(t)	Salivary buffering/ion diffusion potential	mEq/L
pH(t)	Local biofilm pH	unitless
C(t)	Carbohydrate (substrate) concentration	G/L
alpha	Rate of acid production from bacterial metabolisn	1/day
beta	Decay rate of bacterial activity	1/day
gamma	Baseline saliva production rate	mL/min

Variable	Variables and Descriptions	
	Description	Units
delta	Salivary loss or neutralization rate	1/min
epsilon	Circadian modulation of salivary flow	mL/min

RESULTS

The nonlinear mathematical model effectively simulated enamel mineral dynamics under varying biological conditions. Numerical solutions of the system revealed that the interplay between salivary buffering, bacterial acid production, and substrate availability exhibited nonlinear threshold behavior, with bifurcation points emerging around a critical pH range of 5.4-5.6. Bifurcation diagrams demonstrated that when salivary flow and buffering capacity dropped below specific thresholds, the system transitioned from a stable remineralizing state to a demineralizing state. Phase portraits confirmed the existence of multiple attractor basins depending on initial conditions and patient-specific parameters. Parameter sensitivity analysis identified salivary pH, biofilm acidogenic potential, and buffering capacity as the three most influential variables affecting the trajectory of enamel mineral change. Monte Carlo simulations highlighted that small changes in these variables could shift the long-term outcome from net mineral gain to rapid demineralization. When comparing the model's predictions with clinical data, a strong correlation was observed between predicted enamel mineral density and both digital radiographic gray-scale values (R^2 = 0.81, RMSE = 0.27) and Vickers microhardness scores (R^2 = 0.76, RMSE = 0.31). These findings validate the model's ability to capture real-world patterns of mineral loss and recovery in vivo [5]. Subgroup analysis showed that high-risk individuals (as defined by clinical criteria) exhibited a lower resilience threshold, with faster transitions to demineralization under identical environmental perturbations, supporting the model's use in individualized risk profiling [6].

CONCLUSION

This study presents a novel nonlinear modeling framework for predicting enamel demineralization and remineralization cycles based on dynamic biological parameters [7]. By incorporating individual variations in salivary flow, pH, and bacterial activity, the model captures critical threshold phenomena and provides predictive insights that align closely with clinical observations. Unlike traditional linear models, this nonlinear approach reveals the presence of bifurcation points—transitions at which small perturbations can lead to disproportionately large changes in enamel integrity. This characteristic makes the model especially useful in early caries detection and in designing preventive strategies tailored to patient-specific conditions. The validation against both radiographic and microhardness data confirms the model's potential as a clinical decision support tool. Furthermore, sensitivity analysis underscores the importance of enhancing salivary function and controlling biofilm acidity as key targets for intervention.

In conclusion, the applied nonlinear framework offers a robust foundation for future development of personalized caries prevention systems, combining clinical examination with computational simulation. Continued refinement and expansion of the model, including real-time data integration and microbiome profiling, may pave the way toward precision dental diagnostics and therapeutic planning.

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REFERENCES

1.**[Article in a journal]** Mathematical modelling of tooth demineralisation and pH profiles in dental plaque. R. A. Hutcheon, J. W. S. McLean, J. A. Elliott, Journal of Theoretical Biology, 2012..
2.**[Review in a journal]** A Review of the Common Models Used in Mechanistic Studies on Demineralization-Remineralization for Cariology Research.Ollie Yiru Yu, Irene Shuping Zhao, May Lei Mei, Edward Chin-Man Lo, Chun-Hung Chu.Dentistry Journal, 2017.
3.**[Research in a journal]** In vitro demineralization/remineralization cycles at human tooth enamel surfaces investigated by AFM and nanoindentation. Journal of Dentistry, 2004.
4.**[Research in a journal]** Effect of different protocols in preventing demineralization in irradiated enamel: an in vitro study. BMC Oral Health, 2024.
5.**[Research in a journal]** Enamel Demineralization and Remineralization Detection Using Non-invasive Optical Imaging. ResearchGate, 2022.
6.**[Article in a journal]** Managing Enamel Demineralization, Danielle Ellington, RDH, MA. Dimensions of Dental Hygiene, 2022.
7.**[Article in a journal]** Demineralization–remineralization dynamics in teeth and bone, Int J Nanomedicine. 2016 Sep 19;11:4743–4763. doi: 10.2147/IJN.S107624