

COMSOL Digital Twin For Raman–NIR Non-Invasive Glucose Sensing: From Prototype To Validation

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Abstract

Non-invasive glucose monitoring remains difficult because glucose-related optical signals are weak, tissue scattering can obscure the Raman response, and small changes in optical alignment or detector response can affect repeatability. This paper presents a COMSOL-based digital twin for a Phase 1 Raman–NIR sensing platform designed to guide bench development before glucose-solution and tissue-phantom validation. The modeled system uses an 830 nm-class excitation source, Rayleigh rejection, collection optics, selected band-pass Raman spectroscopy (BRS) channels, an APD Raman detector, a reference photodiode, and data-acquisition hardware. The digital twin combines Ray Optics, spectral-response modeling, Heat Transfer analysis, and parameter sweeps. Ray Optics was used to examine the excitation and collection geometry. Spectral-response modeling evaluated Rayleigh rejection and transmission through selected BRS channels near 901.3 nm, 915.5 nm, and 920.15 nm. Heat Transfer modeling estimated sample warming during continuous optical exposure, while Python-based postprocessing demonstrated APD/PD reference normalization, three-band feature extraction, and simulation-guided glucose calibration. The current calibration data are simulation-defined and are intended to test the modeling and processing workflow rather than report measured device performance. The next stage will collect glucose-solution and tissue-mimicking phantom measurements. Measured spectra will be used to refine tissue-scattering assumptions, detector-noise models, filter-response curves, and the calibration workflow. The proposed digital twin reduces trial-and-error prototyping and provides a structured path from optical design to experimental validation.

Keywords: COMSOL Multiphysics, digital twin, Raman–NIR sensing, non-invasive glucose monitoring, Ray Optics, Heat Transfer, band-pass Raman spectroscopy.

1. Introduction

Non-invasive glucose monitoring remains an important research goal because current continuous glucose monitoring systems require transcutaneous sensor insertion and periodic replacement. Although these devices have improved diabetes management, insertion-related discomfort, skin irritation, recurring cost, and reluctance toward long-term use remain concerns [1–3]. Optical sensing offers a potential alternative by examining tissue or fluid samples without repeated blood collection. Raman spectroscopy is particularly attractive because molecular vibrational modes can provide chemically specific information about glucose-related spectral features.

Reliable Raman-based glucose sensing, however, remains difficult. The glucose-related response is weak and can be obscured by tissue scattering, fluorescence, and the much stronger Rayleigh component. Variations in source power, optical alignment, sample position, filter response, and detector sensitivity may further reduce repeatability [1, 4]. Band-pass Raman spectroscopy (BRS) addresses part of this challenge by measuring selected Raman regions rather than acquiring a complete spectrum. A glucose-sensitive center band and adjacent sidebands can support compact detection and local background compensation [4].

The proposed Phase 1 platform uses an 830 nm-class

excitation source, off-axis illumination, collection optics, Rayleigh rejection, three selected BRS channels, an amplified Raman detector, a reference photodiode, and data-acquisition hardware. The reference channel monitors source-power and common-mode coupling variations, while the three Raman channels provide the spectral points required for background-sensitive area and slope calculations. The platform is intended initially for controlled studies using glucose solutions and tissue-mimicking phantoms.

Developing this optical pathway requires coordinated selection of the excitation geometry, lens positions, filter characteristics, detector alignment, reference channel, and operating conditions. Rayleigh leakage, detector displacement, optical losses, and localized sample heating may each influence measurement quality. Evaluating these factors only through physical reconstruction would require repeated component replacement and realignment. A COMSOL-based digital twin provides a practical method for examining these interdependent optical and thermal factors before experimental assembly.

This paper presents a Phase 1 simulation-guided workflow combining COMSOL Ray Optics, spectral-response modeling, Heat Transfer analysis, parameter sweeps, and Python-based APD/PD signal processing. The workflow evaluates the

excitation and collection geometry, three-band spectral response, reference normalization, localized temperature rise, feature extraction, and calibration procedure. The calibration signals are simulation-defined and are used to verify the modeling and processing sequence rather than report measured device performance.

The next stage will use independently prepared glucose solutions and tissue-mimicking phantoms to compare measured and simulated responses, characterize detector noise, and refine the optical, thermal, and calibration models. Successful Phase 1 validation will support later NV-diamond quantum-assisted sensing, optional mid-infrared confirmation, NIR photoplethysmography, and multimodal glucose estimation [5, 6].

2. Related Studies

Non-invasive glucose monitoring has been investigated using optical spectroscopy, near-infrared sensing, photoplethysmography, electromagnetic methods, and wearable physiological signals. These approaches may reduce dependence on invasive or minimally invasive sensors, but their performance remains sensitive to weak glucose-specific responses, tissue variability, motion, environmental conditions, and sensor drift [1–3].

Raman spectroscopy offers molecular specificity but is limited by weak glucose-related signals, fluorescence, tissue scattering, and residual Rayleigh light. BRS reduces optical complexity by measuring selected Raman regions rather than the complete spectrum. Bresci et al. demonstrated that a glucose-sensitive band combined with adjacent sidebands can support local background compensation in a compact sensing configuration [4].

Relevant validation principles have also been demonstrated using other optical modalities. Kaluza et al. evaluated a mid-infrared photothermal system using participant-specific calibration followed by testing in separate sessions [7]. Although mid-infrared absorption differs from Raman scattering, their study emphasizes requirements relevant to both approaches, including repeatable positioning, reference measurements, instrument stability, and separation of calibration and evaluation data.

Recent work has further explored wearable, federated-learning, and quantum-assisted approaches for glucose estimation and biomedical sensing [8–11]. These studies primarily address data-driven prediction, privacy-preserving computation, wearable integration, or future sensing architectures. In contrast, the present work focuses on the preceding physics-based stage: using COMSOL to evaluate the Raman–NIR optical pathway, spectral filtering, thermal behavior, and design sensitivity before bench validation and later multimodal or quantum-assisted extensions [5, 6].

3. System Concept and Digital Twin Workflow

The research is organized into two phases. Phase 1 establishes the Raman–NIR sensing platform and its

COMSOL-based digital twin for studies with glucose solutions and tissue-mimicking phantoms. Phase 2 will build on the validated Phase 1 results by extending the platform toward NV-diamond quantum-assisted sensing, optional mid-infrared confirmation, NIR photoplethysmography, and multimodal glucose estimation. This paper focuses on Phase 1 and examines how the digital twin can guide prototype development and subsequent experimental validation. Figure 1 summarizes the two-phase research pathway.

The Phase 1 sensing platform follows a compact band-pass Raman spectroscopy (BRS) architecture. An 830 nm-class excitation source illuminates a glucose solution or tissue-mimicking phantom. The Raman-scattered light is collected by the optical system, passed through a Rayleigh-rejection filter, and directed to three selected BRS channels. An amplified Raman photoreceiver records the filtered signal, while a reference photodiode monitors variations in the excitation power. The reference measurement is subsequently used to normalize the Raman-channel response.

The spectral model includes three detection windows centered near 901.3, 915.5, and 920.15 nm. The center window represents the glucose-sensitive Raman region, whereas the lower and upper sidebands provide estimates of the surrounding spectral background. Together, these measurements support background compensation and the calculation of a concentration-sensitive Raman metric without requiring acquisition of the complete Raman spectrum [4].

Figure 2 presents the complete Phase 1 development workflow. Clinical and engineering requirements are translated into a virtual optical system defined by the source characteristics, sample properties, filter responses, detector geometry, and operating conditions. The work reported in this paper includes COMSOL Ray Optics modeling, Heat Transfer analysis, spectral-response calculations, parameter sweeps, and Python-based APD/PD signal processing. These analyses examine optical alignment, filter placement, detector coupling, Rayleigh leakage, thermal behavior, and the sensitivity of the calculated Raman metric to changes in the principal design parameters.

The Wave Optics analysis and simulated-versus-measured comparison shown in Figure 2 represent subsequent refinement and validation stages. After measurements from glucose solutions and tissue-mimicking phantoms become available, the experimental results will be used to update the material, filter, and detector parameters in the digital twin. Accordingly, the calibration results presented in this paper are simulation-defined and demonstrate the proposed modeling and signal-processing workflow rather than experimentally validated device performance.

4. COMSOL Modeling Methodology

The Phase 1 digital twin was implemented in COMSOL Multiphysics version 6.4 [12] using the Ray Optics and Heat Transfer interfaces to evaluate the Raman–NIR design

Project Overview: Two-Phase Pathway for Non-Invasive Glucose Monitoring

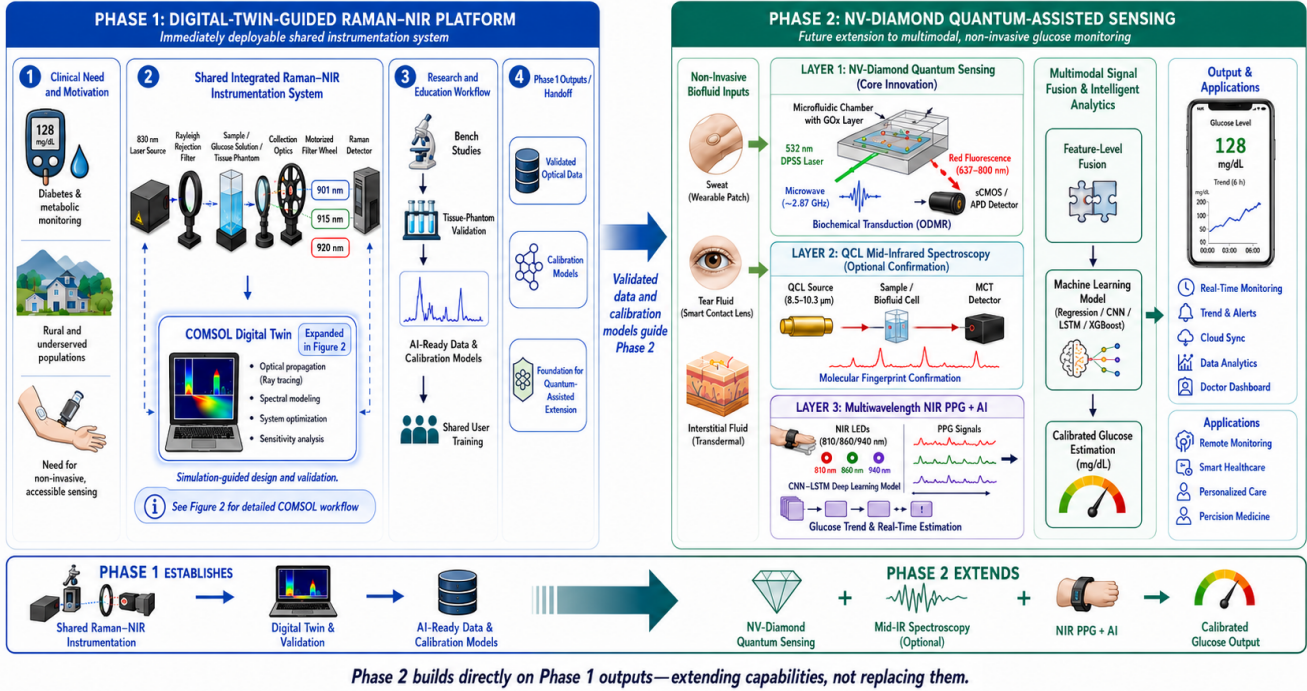


Figure 1: Two-phase pathway for Raman-NIR non-invasive glucose monitoring. Phase 1 develops the COMSOL-guided Raman-NIR platform for bench and phantom validation; Phase 2 extends the validated outputs toward quantum-assisted and multimodal sensing.

before prototype construction. The model examined excitation and collection geometry, Rayleigh rejection, three-band filter selection, detector alignment, and thermal loading. The baseline configuration used 830.35 nm excitation and detection channels centered near 901.3, 915.5, and 920.15 nm. COMSOL parameter sweeps evaluated optical sensitivity, while a separate simulation-defined glucose sweep supported the Python-based normalization and calibration workflow.

4.1. Ray Optics Model

The optical layout was implemented using the Ray Optics interface in COMSOL Multiphysics. The geometry included the excitation source, tissue-phantom region, quartz window, Raman-emission region, collection optics, Rayleigh-rejection filter, three-band filtering stage, focusing lens, Raman detector, and reference photodiode. Figure 3 shows the modeled Phase 1 geometry.

The excitation beam was directed obliquely toward the sample to separate the excitation and collection paths and reduce direct coupling into the Raman detector. Raman rays were launched from the illuminated region, collected approximately normal to the sample surface, and propagated through the collection optics, filters, focusing lens, and detector plane.

The model evaluated ray trajectories, component placement, and detector alignment to guide experimental bench configuration. Because the rays were prescribed rather than generated from a molecular Raman-scattering model, the results represent geometric verification rather than quantitative prediction of Raman intensity.

4.2. Three-Band BRS Filter Model

The band-pass Raman spectroscopy (BRS) model used a lower sideband at 901.3 nm, a glucose-sensitive band at 915.5 nm, and an upper sideband at 920.15 nm. For 830.35 nm excitation, these wavelengths correspond approximately to Raman shifts of 948, 1120–1125, and 1175 cm^{-1} , respectively. The sidebands provide local spectral context for background compensation and feature extraction [4].

The Raman shift was calculated as

$$\Delta\nu = \left(\frac{1}{\lambda_0} - \frac{1}{\lambda_s} \right) 10^7, \quad (1)$$

where λ_0 and λ_s are the excitation and scattered wavelengths in nm, respectively, and $\Delta\nu$ is expressed in cm^{-1} .

The spectral model combined long-pass Rayleigh rejection with Gaussian band-pass transmission. Each BRS response was approximated as

$$T_{\text{BPF}}(\lambda) = \exp \left[-4 \ln(2) \left(\frac{\lambda - \lambda_c}{\text{FWHM}} \right)^2 \right], \quad (2)$$

where λ_c is the filter center wavelength and FWHM is its full width at half maximum. The combined response was defined as $T_{\text{total}}(\lambda) = T_{\text{LP}}(\lambda)T_{\text{BPF}}(\lambda)$. This model examined rejection of the 830.35 nm excitation and Rayleigh component while preserving the selected Raman bands.

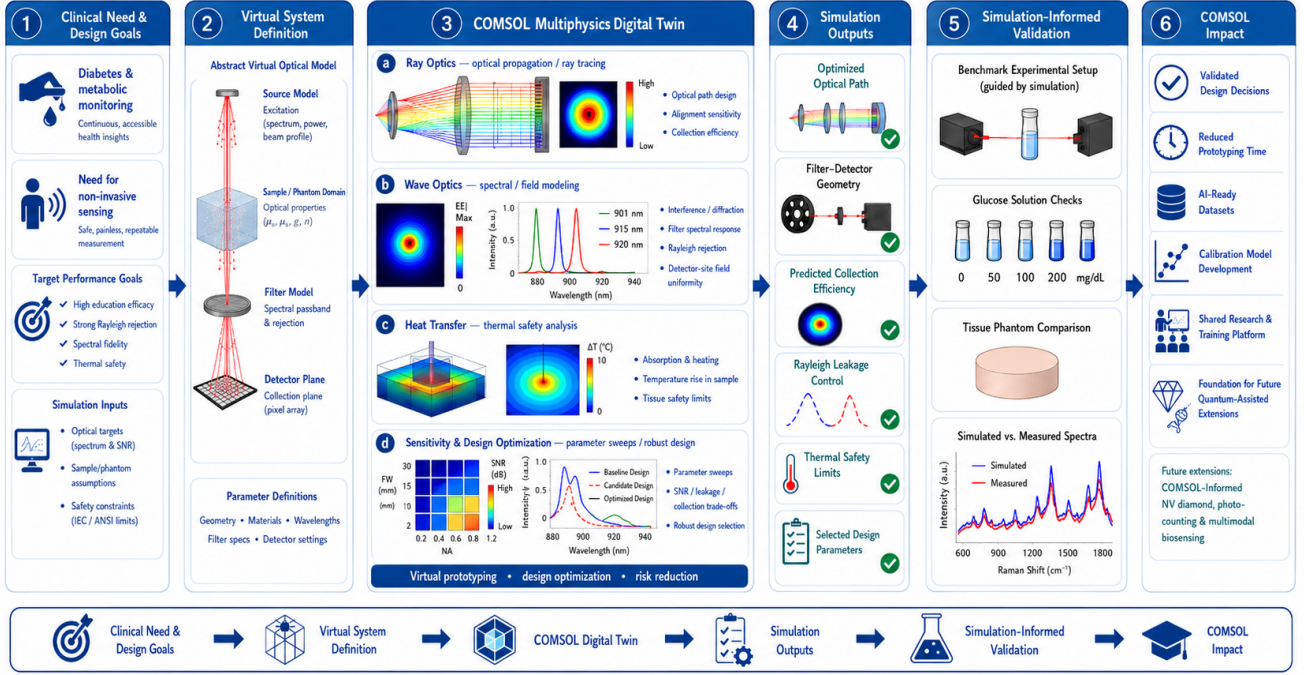


Figure 2: COMSOL-based digital twin workflow for Phase 1 Raman-NIR glucose sensing. The workflow defines the virtual optical system and uses Ray Optics, spectral-response modeling, Heat Transfer analysis, and parameter sweeps to guide glucose-solution and tissue-phantom validation.

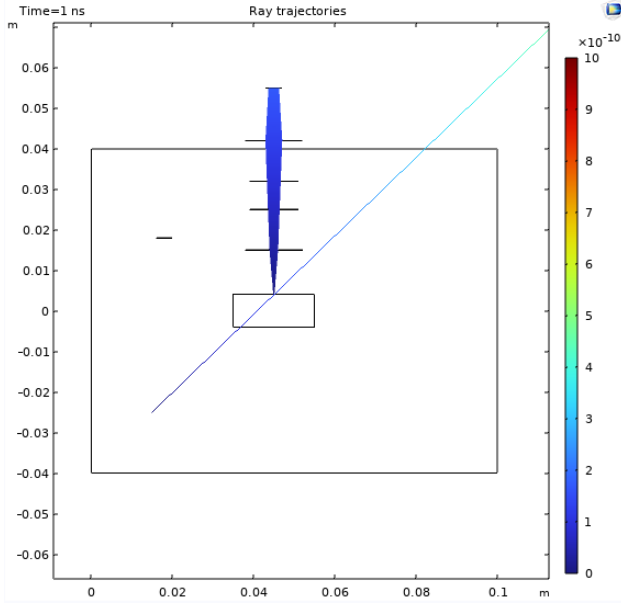


Figure 3: COMSOL Ray Optics model of the Phase 1 Raman-NIR sensing pathway. The off-axis 830.35 nm excitation ray is directed toward the sample region, while Raman emission is collected through the optical path and guided toward the detector plane.

4.3. APD/PD Reference Normalization

The Raman avalanche photodiode (APD) measured the filtered response, while the reference photodiode (PD) monitored excitation-power and common-mode coupling variations. Each BRS signal was corrected using $S_{\text{corr},i} = S_{\text{APD},i}/S_{\text{PD}}$ and bandwidth-normalized as $W_i = S_{\text{corr},i}/\text{FWHM}_i$.

The resulting lower, glucose-sensitive, and upper channel responses were used for area- and slope-based feature extraction. This procedure reduces dependence on absolute signal magnitude but cannot eliminate differential changes caused by positioning, scattering, or detector coupling.

4.4. Heat Transfer Model

The Heat Transfer model estimated localized sample warming during continuous optical exposure. It included the tissue-mimicking sample, quartz window, and localized absorption region. Heat generation was confined to the illuminated volume, with convective cooling applied at the external boundaries. The transient temperature distribution was governed by

$$\rho C_p \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) + Q_{\text{vol}}, \quad (3)$$

where ρ , C_p , and k denote density, specific heat capacity, and thermal conductivity. The volumetric heat source was estimated as

$$Q_{\text{vol}} = \frac{P_{\text{laser}} f_{\text{abs}}}{A_{\text{spot}} d_{\text{heat}}}, \quad (4)$$

where P_{laser} , f_{abs} , A_{spot} , and d_{heat} are the incident power, absorbed fraction, illuminated area, and heating depth, respectively.

The baseline simulation used $P_{\text{laser}} = 91.5 \text{ mW}$, $f_{\text{abs}} = 0.02$, a $0.5 \text{ mm} \times 1.0 \text{ mm}$ illuminated area, a 1 mm heating depth,

and an ambient temperature of 293.15 K. The output was the temperature rise, $\Delta T = T - T_{\text{ambient}}$, after 300 s.

4.5. Parameter Sweeps and Sensitivity Studies

COMSOL sweeps examined optical alignment, filter-center wavelength, and detector position, including lateral detector offsets of -2 , 0 , and $+2$ mm. These studies identified parameters that may affect coupling, repeatability, and calibration stability.

The glucose analysis was performed separately using simulation-defined APD/PD signals from 0 to 500 mg/dL in 50 mg/dL increments. These signals were generated to test the normalization, feature-extraction, repeated-measurement, and calibration procedures in Section 5 and were not obtained from glucose solutions or tissue phantoms.

5. Python-Based Signal Processing and Calibration

Python postprocessing connected the COMSOL-defined sensing configuration with reference normalization, three-band feature extraction, calibration fitting, and error analysis. Because experimental signals were unavailable, this stage used simulation-defined APD/PD measurements.

Two features were calculated from the bandwidth-normalized responses. The first was the absolute triangular area,

$$A = \frac{1}{2} |x_1(y_2 - y_3) + x_2(y_3 - y_1) + x_3(y_1 - y_2)|, \quad (5)$$

where x_i is the Raman shift and y_i is the corresponding normalized response. This feature measures the departure of the three points from a linear background. The second feature was the sum of the absolute local slopes,

$$M_{\text{slope}} = \left| \frac{W_g - W_l}{\nu_g - \nu_l} \right| + \left| \frac{W_h - W_g}{\nu_h - \nu_g} \right|, \quad (6)$$

where W_l , W_g , and W_h represent the lower, glucose-sensitive, and upper channels, respectively, and ν_l , ν_g , and ν_h are their Raman shifts. The area metric characterized the three-point spectral shape, while the slope metric measured local variation around the center band.

The simulated dataset contained 11 glucose levels from 0 to 500 mg/dL, with 10 repeated observations per level. Common source-power drift and detector noise were introduced before APD/PD normalization. A quadratic relationship between the area metric and assigned glucose concentration was then fitted and used to generate predicted values.

Performance was summarized using RMSE, MAE, R^2 , and MARD. The zero-glucose condition was excluded from MARD because its relative error is undefined. Predicted values were also compared with $\pm 15\%$ reference bands. Because calibration and evaluation used observations generated by the same controlled signal model, these metrics characterize workflow consistency rather than independent experimental or clinical accuracy.

6. Results

The Ray Optics simulation established the nominal excitation and collection paths for the Phase 1 Raman–NIR configuration. As shown in Fig. 3, the 830.35 nm excitation beam reaches the sample obliquely, while the simulated Raman rays are collected approximately normal to the surface and directed toward the detector. The model therefore verifies the proposed bench geometry and alignment rather than predicting absolute Raman intensity.

The spectral-response model evaluated separation of the excitation wavelength from the selected Raman channels. Figure 4 shows that the 830.35 nm excitation and Rayleigh component is strongly attenuated by the modeled long-pass stage, while the BRS channels near 901.3, 915.5, and 920.15 nm remain within the detector-side transmission region. Measured filter curves will be required to quantify insertion loss and out-of-band leakage.

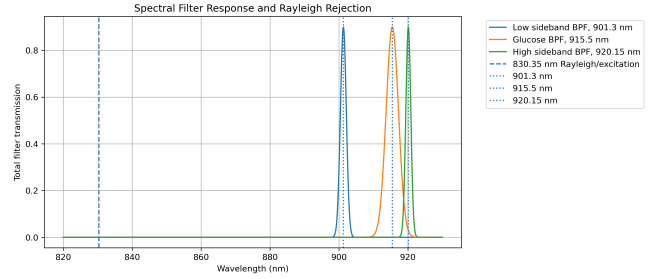


Figure 4: Spectral-response model showing rejection of the 830.35 nm excitation/Rayleigh wavelength and transmission of the selected BRS channels near 901.3 nm, 915.5 nm, and 920.15 nm.

Figure 5 presents the selected channels in the Raman-shift domain. Within the controlled model, the center band exhibits the principal concentration-dependent change, while the sidebands characterize the surrounding response. These three points provide the inputs for the area and slope metrics without relying on absolute APD amplitude alone.

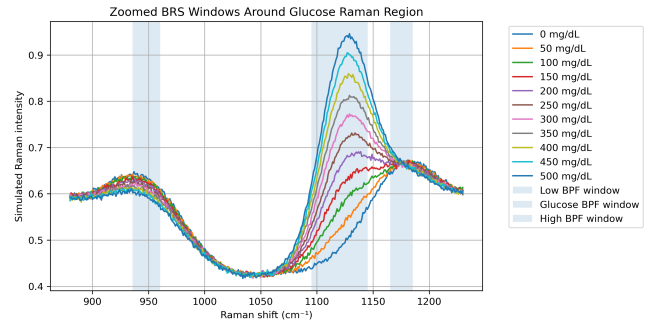


Figure 5: Zoomed simulated Raman response around the selected BRS windows. The shaded regions show the low sideband, glucose-sensitive band, and high sideband used for compact three-band Raman analysis.

The Heat Transfer model estimated localized sample warming during continuous exposure. Figure 6 shows a maximum simulated temperature rise of approximately 0.4 K after 300 s under the assumed laser power, absorption, spot size, and cooling conditions. The rise remained localized near the illuminated region.

This result provides an initial estimate for phantom-stage

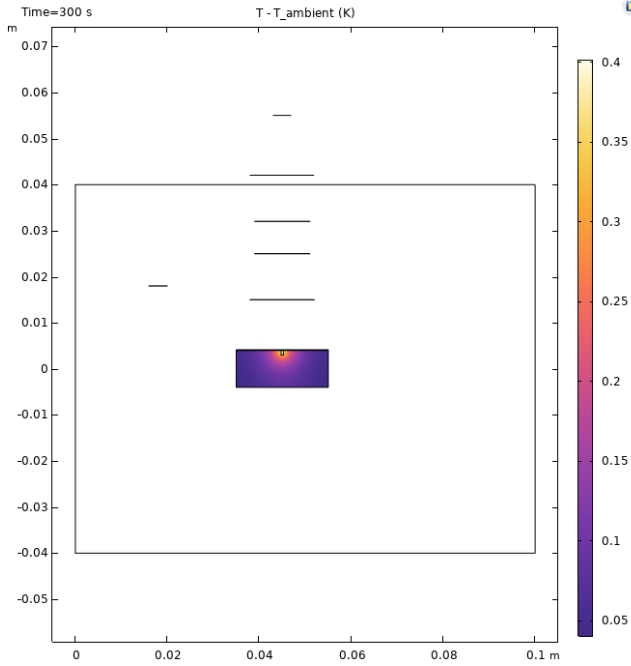


Figure 6: COMSOL Heat Transfer result showing temperature rise after 300 s of simulated optical exposure. The preliminary model estimated a localized maximum rise of approximately 0.4 K.

exposure planning but does not independently establish optical safety. Direct temperature monitoring will therefore be required during experimental validation.

Figure 7 summarizes the optical concept, Raman simulation, three-band extraction, APD/PD normalization, calibration, and predicted-versus-reference comparison. The analysis used 11 glucose concentrations from 0 to 500 mg/dL, with 10 simulated measurements per concentration.

Under the modeled drift and detector-noise conditions, the workflow produced $\text{MARD} = 7.53\%$, $\text{MAE} = 11.83 \text{ mg/dL}$, $\text{RMSE} = 15.77 \text{ mg/dL}$, and $R^2 = 0.990$. Most predictions remained close to the reference line and within the displayed error bands. Because calibration and evaluation used observations from the same controlled model, these values indicate internal workflow consistency rather than independent experimental or clinical performance.

7. Discussion

The Phase 1 digital twin reduces design uncertainty before prototype construction by linking optical layout, spectral filtering, thermal analysis, and signal processing. Ray Optics supports component placement and alignment, while the filter model identifies a pathway for separating the selected Raman bands from the excitation wavelength. The thermal model provides an initial estimate of sample warming, and the Python workflow verifies APD/PD normalization and three-band calibration processing.

These results remain dependent on simplified assumptions. Ray Optics does not reproduce spontaneous Raman generation, fluorescence, multiple scattering, or wavelength-dependent tissue absorption. The filter model also uses idealized

responses rather than measured transmission curves. Consequently, experimental characterization is required to quantify Rayleigh leakage, insertion loss, detector response, and channel overlap.

The three-band BRS configuration reduces hardware complexity by using a glucose-sensitive center channel and two local-background channels [4]. However, three discrete measurements cannot fully characterize fluorescence, overlapping molecular bands, or broad tissue-background variation. Reference normalization may reduce common source fluctuations but cannot eliminate differential changes caused by positioning, scattering, surface contact, or detector alignment.

The simulated performance metrics therefore should not be compared directly with experimental or clinical results. Although the sensing modality differs, the session-separated evaluation reported by Kaluza et al. illustrates the additional variability introduced by instrumental, biological, and session-to-session effects [7]. The present contribution is therefore a testable system design and processing workflow, not evidence of clinical glucose-measurement accuracy.

8. Limitations and Experimental Validation Plan

The principal limitation is that the glucose-dependent signals were generated from a controlled model rather than measured solutions, tissue phantoms, or human participants. Optical and thermal results also depend on assumed filter functions, material properties, absorption, cooling, and noise conditions.

Validation will begin with measurements of source stability, detector dark response, reference-channel variation, filter transmission, Rayleigh leakage, alignment sensitivity, and temperature. Glucose-solution testing will then use independently prepared batches, repeated acquisitions, blank measurements, and blinded concentrations. Tissue-mimicking phantoms will subsequently introduce scattering, absorption, background variation, attenuation, and sample heterogeneity.

Calibration and evaluation measurements will be separated by preparation batch and acquisition session to avoid optimistic results caused by splitting repeated measurements from the same sample. Fixed positioning and repeated reference measurements will further support reproducibility [7]. Measured optical, detector, and thermal data will then be used to update the digital twin. Human-subject evaluation will be considered only after successful solution- and phantom-stage validation.

9. Conclusion

This paper presented a COMSOL-based digital twin for the Phase 1 development of a Raman-NIR non-invasive glucose-sensing platform. Ray Optics assessed the excitation and collection geometry, spectral modeling examined Rayleigh rejection and three-band BRS selection, and Heat Transfer analysis predicted a maximum temperature rise of approximately 0.4 K after 300 s.

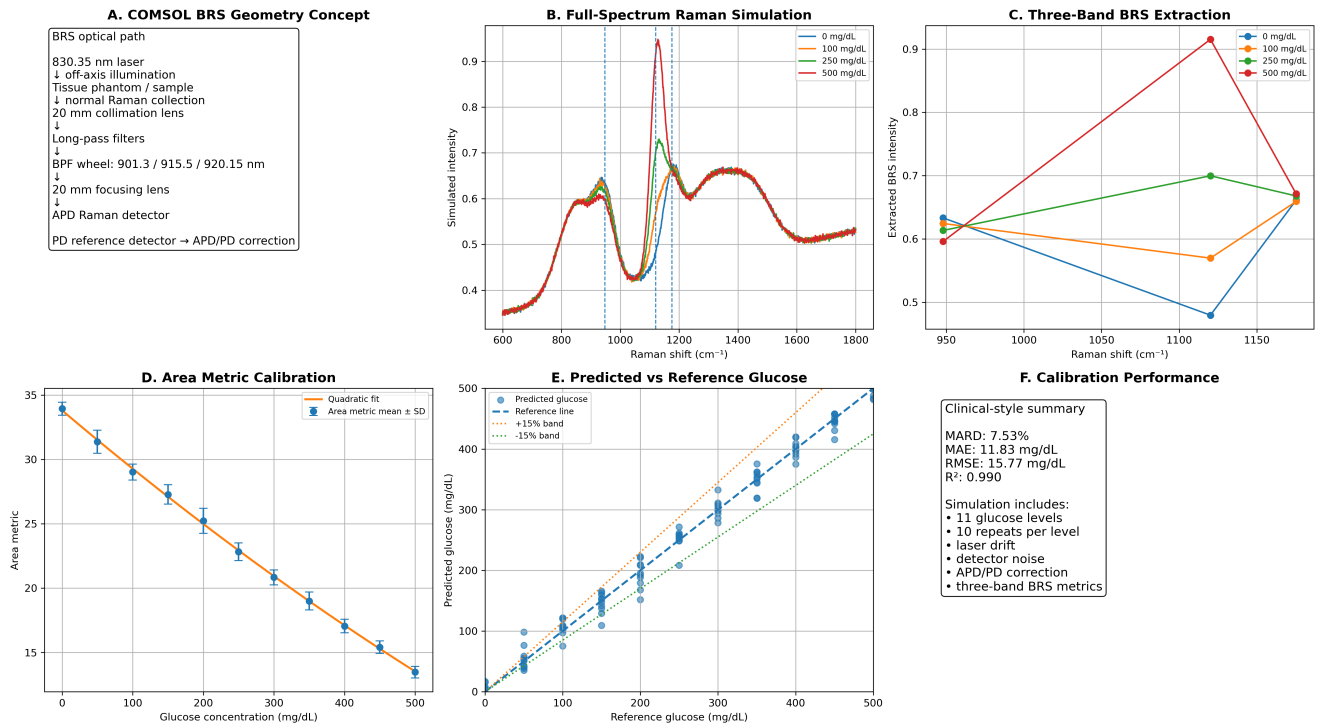


Figure 7: Integrated simulation-guided BRS calibration panel showing the optical concept, Raman simulation, three-band extraction, area-metric calibration, predicted-versus-reference glucose comparison, and performance summary. Results are based on simulation-defined APD/PD signals with modeled drift and detector noise.

Python postprocessing incorporated APD/PD normalization, bandwidth correction, feature extraction, and calibration testing. The controlled simulation produced a MARD of 7.53%, an MAE of 11.83 mg/dL, an RMSE of 15.77 mg/dL, and an R^2 of 0.990. These values demonstrate internal workflow consistency rather than clinical performance.

The next stage will refine the digital twin using independently prepared glucose solutions and tissue-mimicking phantoms, assessing calibration stability across sessions. Successful validation will enable future quantum-assisted and multimodal extensions.

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