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Editorial

Recent Advances in the Application of Mathematical and Computational Models in Biomedical Science and Engineering

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This Special Issue of Bioengineering is dedicated to the development of novel mathematical models for better understanding complex multidisciplinary interactions and processes at the organ, tissue, and cellular scales for different biomedical science and engineering applications, including diagnostic, therapeutic, imaging, and interventional. Ten individual contributions from renowned research groups across the world have been published in this issue.

In the first article of this Special Issue, Khan et al. [1] investigated the biological peristaltic transport phenomena in an asymmetric channel saturated with porous media under the action of an externally applied magnetic field. Finite element based analysis was conducted to quantify the velocity and pressure distributions and bolus trapping for different values of Reynolds number, Hartmann number, and porosity. The model was validated by comparing the predicted results with those available in the previous literature. The study concludes that magnetic field and porosity are useful tools to control the velocity, pressure, and boluses in the peristaltic flow.

Oberleitner et al. [2] proposed a holistic design of experiment (hDoE) method for process development and characterization, which is an iterative approach to experimental design and evaluation that minimizes the number of runs invested while maximizing the overall process understanding in manufacturing processes. To illustrate the validity over a range of scenarios, the proposed method is benchmarked against standard process characterization approaches in a set of in silico simulation studies. The presented results highlight a >50% decrease in the number of experiments utilizing the hDoE approach, even for simple cases. Authors highlighted the application of hDoE in biopharmaceutical manufacturing could result in a substantial reduction of development costs and time to market, ultimately leading to more affordable drugs.

In another study of this Special Issue, Bafakeeh et al. [3] presented an analytical approach to the double diffusion flow of viscoelastic micropolar fluid by utilizing magnetized nanoparticles containing the microorganisms, also accounting for thermophoresis, Brownian motion, and thermodiffusion aspects, along with variable thermal conductivity. The validation of the developed model was done by comparing the simulated solution with previously reported results. This study provides a better understanding of the bioconvective aspect of viscoelastic micropolar nanofluids with several prospective bioengineering applications.

Ghufran et al. [4] presented the application of computer-based drug discovery (CADD) approaches to develop drug-like compounds capable of preventing the replication of SARS-main CoV-2's viral protease M^{pro} (3CLpro). Notably, structure-based virtual database screening, molecular docking, and drug-likeness evaluations of potential

compounds were tested using three databases (ChemBridge, ZINC, and in-house). Molecular dynamics simulation based analysis was conducted to validate the outcomes of structure-based virtual screening. The study identified three most active anti-viral compounds ZINC08535852, ChemBridge63310525, and 12-quinoxaline derivative, that can potentially be employed as a medication to treat SARS-CoV-2 illness.

Xue et al. [5] reported a study related to the modelling and analysis of hybrid transformation for lossless big medical image compression. This study aimed at safe storage, fast image service, and minimum computing power utilizing advanced steganography, wavelet transforms, and lossless compression. Notably, a fast and smooth knight tour algorithm was used to embed patient data into medical images, a discrete wavelet transform was used to protect shield images, and lossless packet compression was used to minimize memory footprints and maximize memory efficiency. The proposed model was tested using 43,752 chest radiographs that comprised 1,00,000 images with relevant details, diagnostic information, and other publicly available datasets. It was found that the expected compression ratio and percentage increased, with a significant reduction in the computational times as compared to other models.

In another study published in this Special Issue, Xue et al. [6] reported the application of deep learning and artificial intelligence for early and accurate detection of COVID-19 and pneumonia. The reported framework utilizes an ensemble learning system based on different deep learning techniques, viz., ResNet152, VGG16, ResNet50, and DenseNet121 that is applied to the large-scale CT scan and X-ray image datasets for identifying COVID-19 and pneumonia. The suggested model outperforms competing approaches and is more efficient than traditional strategies for multi-class categorization of various illnesses.

Huang et al. [7] reported a study that examined the spatial dependence of Electromyography (EMG)–force relations using both simulated and experimental approaches. Notably, the EMG–force relations were examined in the biceps brachii muscles of nine healthy subjects. The findings of this study confirmed the EMG–force relation is sensitive to different motor unit spatial distributions and different proximal–distal electrode positions. The EMG–force relation results presented in this study could serve as a convenient and useful adjunct parameter for assessing muscle or motor unit changes associated with pathology, injury, and aging.

Singh et al. [8] presented a novel application of a near-infrared light-emitting diode (LED) to provide non-invasive acupuncture-like physical therapy. Two commercial LEDs are selected and first characterized to quantify the light irradiation profile, which was utilized in computational modelling and simulations for investigating the heat transfer induced due to light-tissue interaction within the skin tissue. Experimental validation of the developed computational model was also conducted. Furthermore, parametric studies were conducted to investigate the effect of applied power, irradiation duration, and LED distance from the skin surface on the temperature rise attained at different depths. The reported results by the author will be helpful in better understanding the effects of various extrinsic factors on the LED-based heating of skin tissue. These results would pave the way for developing cost-effective and easy-to-use LED-based wearable devices to provide on-demand physical stimulus at home without needing to go to clinics, thus promoting healthy aging.

Raju et al. [9] presented a predictive model for SARS–CoV–2 using machine learning techniques, such as neural networks, decision trees, and random forests. The proposed model integrates stochastic regression, neighbor embedding, and Sammon mapping techniques to enhance the precision and accuracy of predictions. The machine learning based predictive model and findings reported in this research could assist policymakers and healthcare professionals to make informed decisions in effectively managing and controlling the pandemic.

Vitková et al. [10] presented an approach based on the paradigms of the system and control theory for robust control of repeated drug administration. A closed-loop feedback control algorithm was designed to compute the required doses to be administered based

on repeated blood samples. The pharmacokinetic compartmental model developed based on the in-vivo concentration samples was utilized in this work. The authors reported that the closed-loop drug delivery scheme worked better than the fixed-dose protocol. The highlighted potential application of this work was related to the design and development of novel sensors and wearable electronic devices in biomedical engineering for feedback-based drug delivery.

This Special Issue highlights novel findings of the state-of-the-art computational models based on multiscale, multiphysics, data-driven, artificial intelligence, and machine learning approaches in the field of bioengineering. We believe that this Special Issue will provide the readers with ample knowledge and lead to the generation of novel ideas for future advancement in the fascinating field of bioengineering.

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