Design of experimental platform for drug molecular learning and simulation

Jiaqi Xing*, Ding Pan

Wuhan University of Technology, Wuhan, China

*Corresponding author: 297094@whut.com

Abstract: Drug molecule learning and simulation experiment platform is built with B/S architecture, which can complete the simulation of pharmacy experiments directly on the web side, aiming to integrate modern science and technology such as artificial intelligence and virtual display with pharmacy molecule research and learning, and facilitate the simulation of pharmacy experiments and the learning of pharmacy knowledge.

1. Introduction

In the 21st century, the development of the Internet is being paid more and more attention to, relying on the Internet to achieve a lot of information interaction, so that people can quickly locate the key information they need in the complex and numerous information, which enables people to achieve a more efficient effect when receiving information.

In this context, this thesis intends to build and design a web page about a drug learning related biomolecular simulation cloud platform, introduces the background and significance of the study of this web system, analyzes the necessity of building a platform web page through a demand survey, and also analyzes the feasibility of the studied system, determines the functions of the website from the perspective of the users and administrators of the drug molecular learning website, and then The functional module design and use case description design of the website were carried out, and some of the functions of the website were elaborated and analyzed.

The website is proposed to be developed in c# language, and Visual Studio 2019 is used as the development platform combined with database to realize the information management functions for users and administrators.

2. Background of website construction

2.1 Application prospect analysis

It is understood that the General Office of the Ministry of Education of China, in order to promote the deep integration of information technology and experimental teaching in higher education, decided to carry out the construction of a model virtual simulation experimental teaching project in ordinary undergraduate higher education schools. The virtual simulation experimental teaching method integrates cutting-edge technologies such as artificial intelligence and virtual reality, and

integrates the science and technology of the new era into the teaching and learning of theoretical knowledge and experimental operation practice and examination of science, medicine and other disciplines. Therefore, the establishment of simulation platform for learning caters to the national policy and has good application prospects.

2.2 User Needs Research

At the beginning of the project, a survey was conducted mainly for pharmacology researchers, one was to investigate the references commonly used by pharmacology research learners when conducting drug analysis, and also to understand their needs in order to better build a platform to meet the needs of pharmacology researchers. This project mainly conducted interviews and surveys on two groups, one is learners who are studying drug pharmacology, among which students are the main group, they are also the backbone of future pharmacological analysis, and they are in the era of rapid development of the Internet, they also have better acceptance of the platform learning, understanding their needs is conducive to designing the platform to make it have better application prospects; one is some pharmacological scholars who have rich experience in Pharmacy scholars, through their survey, to consider the source of data analysis of the platform and the design of the standardization. During the survey, we got the information that many respondents are willing to register and use such a simulation learning platform if it is available, which also shows the importance of establishing a relevant platform.

3. Technology related to drug learning website design

The experiment platform adopts B/S architecture, with the server as the core of the system function implementation, only in the Web browser can carry out the relevant operations of the platform, without the need to install another client. At the same time, the B/S architecture is highly interactive, which is ideal for building online communication and sharing websites. This thesis will analyze the B/S architecture to verify the feasibility of building the platform.

B/S architecture is a browser-server architecture, where the main transaction logic of the system is implemented on the server side and the system only needs to be operated on the web browser. In B/S architecture, Web and WebApp are responsible for display logic and transaction processing respectively, which reduces the pressure on the client side. Moreover, since B/S runs directly on WAN, only the server needs to be upgraded to complete the upgrade of the system, which is low cost and highly distributed, suitable for application to systems facing a large user base.

4. Specific design of the drug learning website

4.1 Functional Design

The home page of the website mainly consists of the registration portal, the drug molecule learning portal and the simulation experiment portal. After registering at the registration portal, you can learn the platform resources and simulate experiments after becoming a registered user.

The registration portal plays the role of displaying the main functions of the website and attracting users with a distinctive and beautiful UI. After users open the website, they first see the display interface of the main functions of the system, i.e. work display and product display. The home interface has a rotating display of platform introduction, navigation bar and content display, etc. The navigation includes: home page, latest research in related fields, drug molecule learning section, simulation and simulation experiments, related database, registration and background, etc.

The drug molecule learning section mainly integrates books related to drug molecule learning,

enters them, searches them by keywords, and uses algorithms to display the most relevant chapters.

The simulation experiments are designed by using the existing research results and input and output feedback in the database, so that the registered users can learn and understand drug molecules more intuitively. The simulation module is designed to simulate the color and state of the material (powder, granules), and to simulate the effect of the experiment, such as reaction time. After the user inputs the relevant operations, the system calls up the internal reaction information and provides feedback on the reaction duration and the changes in each phase.

4.2 Database system design

4.2.1 Identify business participants

The scope and boundaries of the system are refined and further defined by focusing on the participants of this learning and simulation experimentation platform. The participants determine the completeness of the system requirements. By identifying participants after completing the use case model, these participants can validate the use cases. We identified the following list of participants, which are divided into two main categories: users and platform staff. The users are divided into unregistered users and registered users, unregistered members are users who have not completed registration, registered members are registered users of the drug molecule learning and simulation experiment platform who have completed registration, unregistered users can be transformed into registered members by registering an account; platform staff are divided into platform administrators, learning module designers, user information administrators, simulation experiment module designers, platform The platform administrator is the manager of the learning and simulation experiment platform and issues notices and announcements; the learning module designer is responsible for the design and construction of the learning subsystem; the user information administrator is responsible for handling user registration and the identity authentication department; the simulation experiment module designer is responsible for the design and construction of the simulation experiment subsystem.

4.2.2 Simulation experiment module use case description

Based on the above, the construction of the participant use case model is carried out. The content of the participant use case model is shown in the functional design module description, which is omitted here, after which the use case description is carried out and the business requirement description is recorded. After the main business participants and other participants of each use case are determined, the use case description can be built.

Table 1: Description of the extended use case for the simulation experiment

Use Case Name	Simulation experiments	Use Case Type:
Use Case ID	ES-02	Business Requirements: ☑
Priority		
Key Business Players	Registered Users	
Other Participants	Simulation experiment department, user information manager	
Other interested associates	Platform Administrator	
Description	This use case describes a registered user conducting a simulated drug experiment in the system	
Pre-requisites	Users must have registered an account and completed a login.	
Triggers	The use case is triggered when the user submits a reservation request.	
Typical event process	Participant Movement	System Response
	Step 1: The user selects the experiment type as well as the experiment material Step 5: The user determines the simulation experiment information. Step 7: User determines the experimental results	Step 2: The system verifies that the user is eligible for the experimental module. Step 3: The system verifies that the material selected by the user is in the experiment database. Step 4: The system confirms the length of time consumed by the user's selected experiment and sends it to the user. Step 6: The system calls the relevant experimental information in the library and outputs it through pictures, videos, etc. and sends the results to the user. Step 8: The system records the simulation experiment information.
Alternative Event Process	Alternative step 3: If the material selected by the user is not in the library, the user is notified and prompted to resubmit. Alternative step 5: If the user chooses to modify the information, the system re-calls the experiment time consuming and other information back to the user. Alternative step 3: If the material selected by the user is not in the library, the user is notified and prompted to resubmit.	
Conclusion	The use case ends when the logged-in user receives an end-of-experiment alert message.	
Post-condition	The user's experiment results are recorded by the system for the next viewing	
Business Rules	Only the relevant experiments entered by the database can be simulated.	
Implementation constraints and descriptions	To provide users with a simulation experiment portal as well as an experiment information selection portal.	
Assumptions	Will be recorded in the personal information experiment.	

5. Conclusions and outlook

5.1 Conclusions

In this era of rapid development and popularity of the Internet, online communication sites have become mainstream, and the B/S architecture, because of its own characteristics, is more suitable for building platforms for a large user base, and can also better meet the needs of online platforms for online communication and sharing. As an online learning platform, the drug molecule learning and simulation experiment platform meets the needs of pharmacy-related students, scholars, and practitioners, facilitates pharmacy research and learning, and caters to national policies, and is a website with development potential that meets the needs of industry-related personnel and is in line with the development of the times.

The drug molecule learning and simulation experiment platform studied in this thesis was developed based on verifying the feasibility of the relevant, investigating the actual needs of users and reviewing a large amount of literature and drawing on a large number of platforms. The module design within the website also considers user-oriented, convenient operation for administrators and

fits the actual development logic situation.

This website integrates the functions of simulation experiment, knowledge sharing, knowledge learning and data integration, which is a complete system that satisfies most of the operations that users want to implement in the website, and at the same time, they can easily view and operate their experiments and user information with one click, which is simple and fast, and very much meets the standard of interactivity.

5.2 Outlook

Although the website designed in this paper has perfect operation functions, there are still some problems in some functions and design of this website due to the limitation of technical level. Therefore, I will continue to learn more and present a more professional and beautiful website in terms of overall design and functional modules implementation. I have the following ideas for the subsequent improvement of the website.

(1) Beautify the interface display, increase the design elements and overall coordination, improve the interesting and beautiful degree of the website.

(2) To make the experiment-related settings more in line with the actual operation, more in line with the experimental operation process.

(3) Optimize the data integration part of the platform, so that the system can retrieve more data.

References

[1] Liu Ning. On website UI design and user experience [J]. Science and Technology Perspectives, 2015(32): 110-111.

[2] Liu Huanjie. The design and implementation of website group system in colleges and universities [J]. Wealth Today, 2021(18): 103-105.

[3] Mu Weiwei, Guo Pengbo. Design and implementation of interactive intelligent art picture website[J]. Electronic Technology and Software Engineering, 2021(21): 96-98.

[4] MING Xiaobo, QIU Huiling, LI Dan. Design and implementation of high-performance portal and its information publishing system [J]. Popular Standardization, 2021(09): 87-89.

[5] Zhang Weiqiang. Development and implementation of dynamic libraries in C++ calling C# [J]. Computer programming skills and maintenance, 2020(01): 50-51+67