

Application of Computer Simulation Teaching Method in the Principles of Chemical Engineering Course: Taking Fluid Transportation as an Example

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Abstract:

Taking fluid transportation as an example, this paper explores the application of computer simulation teaching methods in the Principles of Chemical Engineering course. On the one hand, it simplifies the calculation process and improves the accuracy of calculations; on the other hand, it stimulates students' learning initiative and cultivates their ability to solve engineering problems by simulating some engineering cases.

Keywords:

Computer simulation
Principles of Chemical Engineering
Fluid transportation

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1. Introduction

Principles of Chemical Engineering is a core course for chemical engineering and technology majors, and it is crucial for cultivating students' engineering application abilities. The course content covers momentum transfer, heat transfer, and mass transfer, laying a foundation for future industrial practice for chemical engineering students^[1-3]. With the advancement of technology, computer simulation has been widely used in industrial practice. Currently, the most commonly used process simulation software in the chemical industry includes Aspen Plus, ChemCAD, PRO/II, and HYSYS^[4-8].

Adopting computer simulation as an auxiliary teaching method can simplify calculations, improve efficiency, and stimulate students' learning initiative.

Most of the materials involved in chemical engineering processes are fluids, and most of them are in a flowing state. It can be said that fluid flow is the foundation of the Principles of Chemical Engineering course. To cultivate students' engineering application abilities, this article takes fluid transportation in the Principles of Chemical Engineering course as an example to explore the application and practice of computer simulation in teaching.

2. Engineering case study

Based on computer simulation, engineering case studies have been conducted in many domestic engineering colleges^[9]. Through engineering case studies, the engineering application abilities of chemical engineering and technology students can be improved. This article selects an engineering case study of fluid transportation:

A chemical plant transports water with a volumetric flow rate of 100 m³/h, a temperature of 35°C, and a pressure of 350 kPa through a $\phi 89 \times 4$ mm pipeline (with an inner wall roughness of 0.06 mm) to the destination. The pipeline is laid 15 m east from the starting point, then 10 m north, elevated 3 m, and finally laid 20 m west to reach the destination. Calculate the pressure loss during the entire process.

In this case study, Aspen Plus software is used for simulation, and the equipment selection is PIPELINE under pressure changer, which represents the pipeline system. The process flow diagram is shown in **Figure 1**. The pipeline system PIPELINE is used to simulate a pipeline composed of multiple segments of pipes with different diameters or inclinations connected in series. When calculating pressure drop and liquid residence time, multiple liquid phases (such as oil and water phases) are treated as a single uniform liquid phase. If there is gas-liquid flow, the pipeline system PIPELINE can calculate liquid retention and flow status. The pipeline system PIPELINE assumes that the fluid flow is one-dimensional, steady-state, and uniform. That is, the influence of the inlet is not considered during simulation, and the flow direction can be horizontal or angled. The fluid temperature distribution can be specified or calculated through heat transfer^[10,11].



Figure 1. PIPELINE module process flow diagram

3. Simulation process and teaching research discussion

Based on Aspen Plus software, the fluid flow process is simulated and calculated. The component addition is simple, with only a single water component. The physical property method adopts the STEAM-TA equation, and

the flow basis (Flowbasis) is selected as Std Vol. Set the feed conditions: input feed (FEED) temperature of 35°C, pressure of 350 kPa, and volumetric flow rate of 100 m³/h.

Next, enter the equipment setting interface. Input the PIPELINE module structural parameters, select “Calculate outlet pressure” for the calculation direction (Calculation direction), choose “Enter node coordinates” for the segment geometry (Segment geometry), and for the thermal options (Thermal options), we assume that the pipeline system does not exchange heat with the outside, so select “Constant temperature” (Specify temperature profile/Constant temperature). For property calculations (Property calculations), select “Do flash at each step,” and for the pipeline flow basis, choose “Use inlet stream flow” as shown in **Figure 2**.

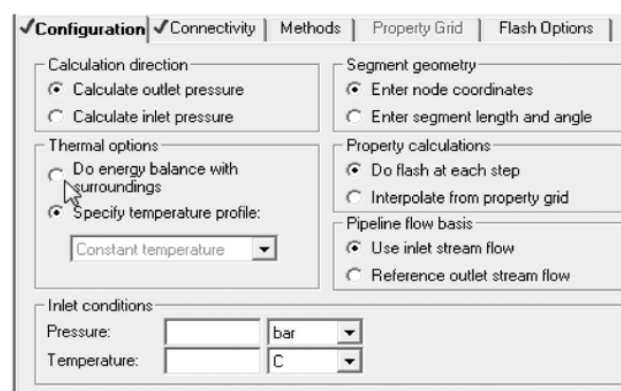


Figure 2. Structural parameters of the PIPELINE module

For the pipeline system equipment calculation, select “Liquid-Only” as the valid phase (Valid phase), as shown in **Figure 3**.

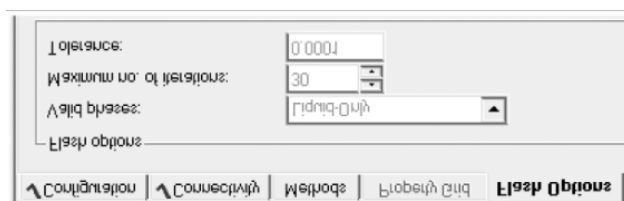


Figure 3. Valid phase of the PIPELINE module

Click N to enter the Blocks / PIPELINE / Setup / Connectivity page and set the connection parameters between each segment of the PIPELINE module. Due to the complexity and diversity of pipeline turns in this case, a schematic diagram related to direction and coordinates is drawn here to facilitate students’ understanding, as shown in **Figure 4**.

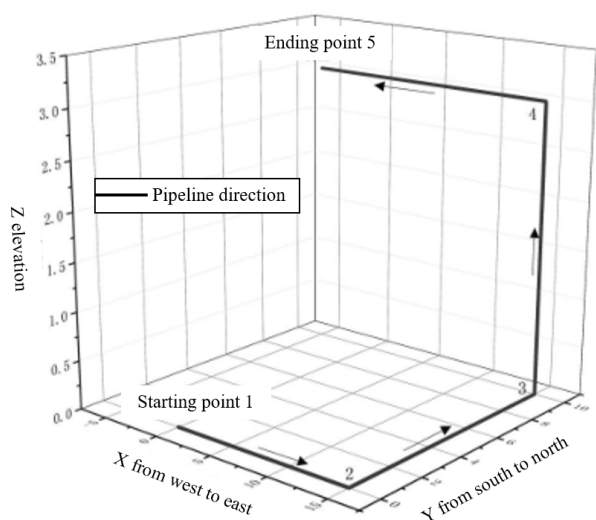


Figure 4. Schematic diagram of pipeline direction

In **Figure 4**, the positive direction of the X-axis represents east, the positive direction of the Y-axis represents north, and the Z-axis represents elevation changes. There are a total of four pipe segments in **Figure 4**, including a total of five nodes including the starting point and ending point. We set the starting point at the coordinate origin (0,0,0), counted as node 1; the pipeline is first laid 15 m east from the starting point, reaching node 2 with coordinates (15,0,0); then laid 10 m north, reaching node 3 with coordinates (15,10,0); then the elevation is raised by 3 m to reach node 4 with coordinates (15,10,3); finally, it is laid 20 m west to reach the ending point 5 with coordinates (-5,10,3).

Based on this reference coordinate system, define the pipe segments and node coordinates in PIPELINE. For pipe segment 1, set the coordinates of node 1 and node 2, as well as input the inner diameter of 81 mm and the inner wall roughness of 0.06 mm for pipe segment 1. The setting method is shown in **Table 1**. The definition of other pipe segments and nodes follows the same approach.

Table 1. Parameter settings for pipe segment 1 in the PIPELINE module

Pipe segment 1	Inlet node 1	Outlet node 2
X-coordinate (m)	0	15
Y-coordinate (m)	0	0
Elevation (m)	0	0
Pipe diameter (mm)		81
Pipe wall roughness (mm)		0.06

After defining the pipeline connections, one can run the simulation and check the control panel. If there are no errors or warnings, it means the final calculation is complete. Then, the results can be viewed as shown in **Table 2**. Since we assumed earlier that the pipeline does not exchange heat with the outside, the outlet temperature of the pipeline remains at 35°C, and the final outlet pressure of the pipeline is 157.81 kPa. Throughout the process, both material and heat balances are conserved. The total pressure loss during the entire fluid transportation process is $350 - 157.81 = 192.19$ kPa, which also illustrates that during long-distance fluid transportation, due to resistance losses and changes in elevation, it is necessary to continuously use transportation machinery such as centrifugal pumps to increase the pressure.

Table 2. Calculation results of the PIPELINE module

Name	Calculation results	Name	Calculation results
Inlet pressure (kPa)	350	Outlet enthalpy (kW)	-438704.37
Inlet temperature (°C)	35	Molar flow rate (kmol/h)	5540.17
Inlet enthalpy (kW)	-438699.58	Mass flow rate (kg/h)	99807.65
Outlet pressure (kPa)	157.81	Thermal load (kW)	-4.78
Outlet temperature (°C)	35		

4. Conclusion

Through computer simulation of this case, students have gained a clearer understanding of Bernoulli's equation, mechanical energy balance, and resistance loss calculations. Real industrial production is far more complex than the examples presented in textbooks. In this case, the pipeline transports fluid not just in one direction or at one elevation, but sometimes even with varying pipe diameters. If one were to rely solely on textbook formulas, the calculation workload would be extremely heavy. The introduction of computer simulation teaching methods into the Principles of Chemical Engineering course has simplified the calculation process and improved accuracy on one hand, and stimulated students' learning initiative on the other. Through training using this case, students can initially solve some simple engineering problems.

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Disclosure statement

The authors declare no conflict of interest.

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