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Composition and Injection Rate Co-Optimization Method of Supercritical Multicomponent Thermal Fluid Used for Offshore Heavy Oil Thermal Recovery

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Abstract: Supercritical multicomponent thermal fluid injection is a new technology with great potential for offshore heavy oil thermal recovery. In the process of thermal fluid generation, the reaction conditions including temperature, pressure, and the organic mass concentration in the reaction material will significantly affect its composition and injection rate and will further affect the thermal recovery and development quality of heavy oil. However, there is a lack of relevant research on the variation rules and control methods of the composition and injection rate of supercritical multicomponent thermal fluids, resulting in a lack of technical mechanisms for effective optimization. To fill this gap, a reaction molecular dynamics simulation method was used to simulate thermal fluid generation under different temperatures, pressures, and organic mass concentrations. The changes in thermal fluid composition and yield with reaction conditions were studied, and a control model of thermal fluid composition and yield was established. The proportional relationship between the thermal fluid generation scale of an offshore heavy oil platform and the simulated thermal fluid generation scale is analyzed, and a collaborative optimization method of thermal fluid composition and injection rate in field applications is proposed. The results show the following: (1) The higher the mass concentration of organic matter, the higher the content of supercritical carbon dioxide and supercritical nitrogen in thermal fluids, and the lower the content of supercritical water. (2) The higher the temperature and pressure, the higher the thermal fluid yield, and the higher the organic mass concentration, the lower the thermal fluid yield. (3) The component fitting model conforms to the power function relationship, and the coefficient of determination R^2 is greater than 0.9; the yield fitting model conforms to the modified inverse linear logarithmic function relationship, the determination coefficient R^2 is greater than 0.8, and the fitting degree is high. (4) The ratio between the actual injection rate of thermal fluids in the mine field and the molecular simulated thermal fluid yield is the ratio of organic matter mass in the platform thermal fluid generator and organic matter mass in the simulated box. (5) Based on the composition and yield control model, combined with the simulation of the ratio relationship between yield and injection rate in the field, a collaborative optimization method of thermal fluid composition and injection rate was established. The research results can provide an effective technical method for predicting, controlling, and optimizing the composition and injection rate of supercritical multicomponent thermal fluids.

Keywords: supercritical multicomponent thermal fluids; offshore heavy oil thermal recovery; supercritical multicomponent thermal fluid composition; supercritical multicomponent thermal fluid yield; co-optimization; molecular dynamics simulation

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1. Introduction

Supercritical multicomponent thermal fluids (scMCTF) are an innovative heat carrier used for thermal recovery of offshore heavy oil. They consist of supercritical water (scH_2O), supercritical carbon dioxide ($scCO_2$), and supercritical nitrogen (scN_2), offering superior heat-carrying, oil-solubilizing, viscosity-reducing, and pressure-maintaining properties. Compared to traditional steam and conventional multicomponent thermal fluids, scMCTFs significantly enhance the recovery rate of heavy oil [1–4]. Additionally, waste fluids produced from oil wells can be used as feedstock to generate scMCTFs, allowing the generation system to be self-sustaining without external energy inputs [5,6]. Due to its notable advantages in enhancing recovery efficiency and reducing costs, scMCTF injection is widely regarded as one of the most promising and valuable next-generation thermal recovery technologies for offshore heavy oil. It also has potential applications in onshore heavy oil fields [7,8].

The typical principle behind scMCTF generation involves gasification and oxidation reactions of organic matter in a supercritical water environment [9]. Reaction conditions influence the composition and yield of scMCTFs, which in turn determine the physical properties of the thermal fluid and the rate at which the scMCTF is injected from offshore platforms into reservoirs. The properties and injection rate of scMCTFs are key factors affecting the effectiveness of thermal recovery [10,11]. Therefore, it is critical to study how scMCTF composition and yield vary with reaction conditions and to establish a control model that enables precise adjustment of scMCTF composition and yield. This will help optimize the parameters for scMCTF injection, improving the quality of offshore heavy oil recovery.

Currently, research on scMCTF injection for heavy oil recovery is scarce, with related studies mainly emerging in the past three years [1–9,12]. No reports have been found on control models or optimization methods for scMCTF composition and yield, highlighting the lack of effective technical approaches. In this context, molecular dynamics simulations are employed to study scMCTF composition and yield under varying temperatures, pressures, and feedstock concentrations. The goal is to establish a control model for scMCTF composition and yield, analyze the relationship between the scale of scMCTF generation in offshore platforms and simulation results, and propose methods to optimize both the composition and injection rate of scMCTFs in field applications. These research findings aim to provide effective technical methods for predicting, controlling, and optimizing scMCTF composition and injection rates, offering crucial technical support for parameter optimization in future offshore heavy oil development projects.

2. Reaction Molecular Dynamics Simulation Model

2.1. Modeling System

Based on the Materials Studio platform for atom or molecule system construction, optimization, and simulation, a multicomponent diesel molecular model was constructed using paraffins, cycloalkanes, monocyclic aromatics, and bicyclic aromatics as model compounds [13], and the ratio of paraffins, cycloalkanes, monocyclic aromatics, and bicyclic aromatics molecules number is 5:3:1:1.

Subsequently, after fixing the number of organic molecules, different numbers of water molecules were added to establish reaction systems with varying organic concentrations, followed by molecular geometry optimization. The organic concentration in the system ranged from 8.39% to 25.14% (Figure 1). Reaction systems with higher organic concentrations have fewer water molecules, fewer total molecules, and looser molecular arrangements.

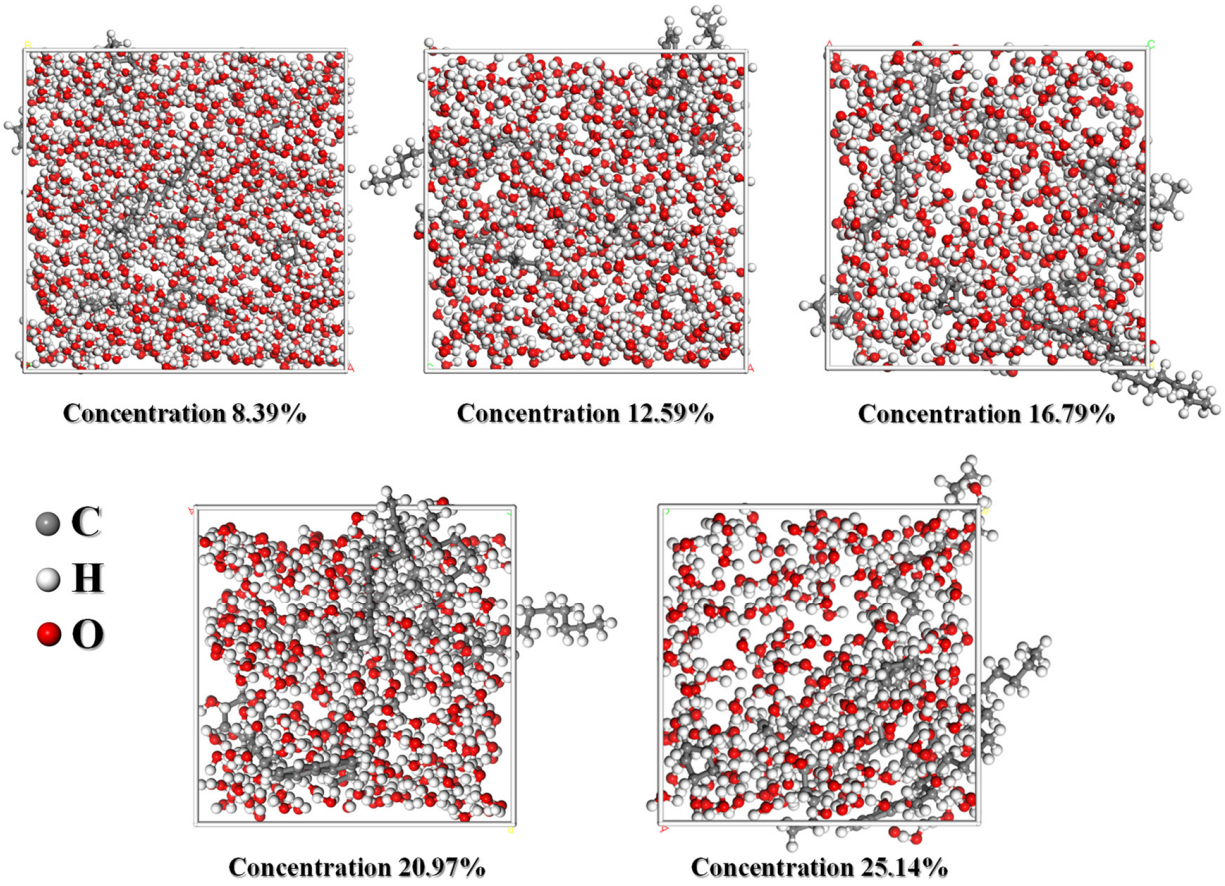


Figure 1. Concentration reaction system.

2.2. Simulated Force Field and Program Setup

The reactive molecular dynamics simulations were carried out using the LAMMPS (Large-scale Atomic or Molecular Massively Parallel Simulator) platform. The ReaxFF reactive force field applied was the C/H/O force field proposed by Chowdhury and van Duin in 2017 [14], which has been widely utilized for simulating the combustion, pyrolysis, and gasification of organic compounds under supercritical water conditions [15–17]. The global simulation time step was set to 0.1 fs, and the simulation procedure included the following steps: ① Charge equilibration using the QEQ method. ② System energy minimization via the conjugate gradient method. ③ Random initialization of atomic velocities at 200 °C according to the Maxwell–Boltzmann distribution. ④ System relaxation under specified temperature and pressure based on the NPT ensemble using the Nose–Hoover method to control temperature and pressure, with damping coefficients 100 times and 1000 times the time step for temperature and pressure, respectively. The relaxation time was 10 ps, allowing the system to reach equilibrium. ⑤ Resetting of the time step after removing the ensemble setting. ⑥ Reaction simulation of supercritical multicomponent thermal fluids using the NPT ensemble, with the reaction temperature and pressure set according to simulation settings. The damping coefficients for temperature and pressure remained unchanged. ⑦ Output and recording of system parameters such as temperature, pressure, system volume, and atomic positions every 100 time steps, along with the storage of product information.

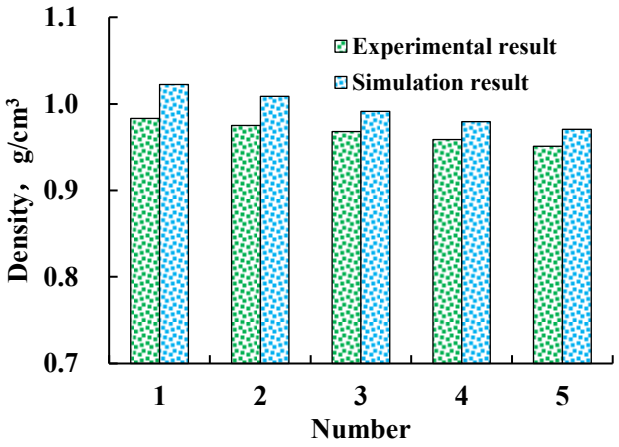
2.3. Model Verification

Based on the different organic matter concentration reaction systems established, the molecular simulation software LAMMPS 64-bit 2Aug2023-MSMPI was used to calculate the system's density. Additionally, molecular simulations of supercritical multicomponent thermal fluid (scMCTF) generation were performed under varying temperatures

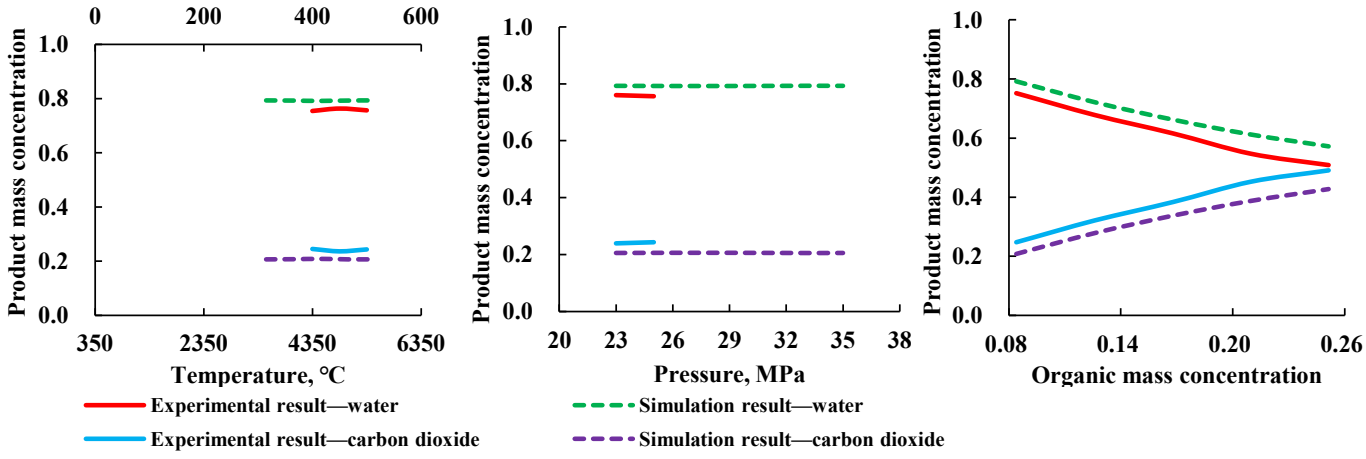
(3500–5500 °C) and pressures (23–35 MPa). Physical experiments were also conducted under real laboratory conditions for systems with the same organic matter concentrations, covering temperatures (400–500 °C) and pressures (23–25 MPa).

In reactive molecular dynamics simulations, reaction temperatures are typically elevated to accelerate reaction rates because the simulation timescales are often on the order of picoseconds (ps) to nanoseconds (ns) [18,19]. According to the Arrhenius equation describing the relationship between reaction temperature and reaction rate [20], scholars such as Voter and SΦrensen introduced the Temperature-Accelerated Dynamics (TAD) method to increase the simulation temperature, which speeds up the reaction process without significantly affecting the reaction mechanisms [21]. This method has been widely applied and validated [22–24]. Therefore, the simulation temperatures in this study were set higher than those in the physical experiments.

A comparison of the simulation and experimental results (Figure 2) shows that the densities of the simulated and measured reaction systems were similar. Furthermore, the mass concentrations of products generated under different reaction pressures, temperatures, and organic matter concentrations from the simulations were numerically close to those obtained from the physical experiments, with highly consistent trends. Therefore, it can be concluded that reactive molecular dynamics simulations can accurately reflect the actual scMCTF generation process.



(**a**) Comparison of reaction system density



(**b**) Comparison of product mass concentration under different reaction conditions

Figure 2. Comparison of molecular dynamics simulation results and experimental results.

3. Change Law of scMCTF Composition and Yield

Based on the established reactive molecular dynamics model, a simulation study of the supercritical multicomponent thermal fluid (scMCTF) generation process was conducted. The simulation parameters were set as follows: a temperature range of 3500 °C to 5500 °C with a step size of 500 °C; a pressure range of 23 MPa to 35 MPa with a step size of 3 MPa; and an organic matter concentration range of 8.39% to 25.14%, with a step size of 4.20%. In total, the reactive molecular dynamics simulations included 125 sets of conditions (5 × 5 × 5).

3.1. Change Law of Composition

Based on the mass concentrations of each component in scMCTF generated under different temperatures, pressures, and organic matter concentrations in the feedstock (Figure 3), the component concentration–temperature–pressure surface for different organic matter concentrations is essentially flat. This indicates that the composition of scMCTF does not significantly vary with temperature and pressure, meaning that temperature and pressure are not the primary controlling factors for scMCTF composition. However, the concentration of organic matter in the feedstock has a greater impact on the composition of scMCTF. As shown in Figure 3, the concentrations of $scCO_2$ and scN_2 increase with the rise in organic matter concentration, while the concentration of scH_2O increases as the organic matter concentration decreases.

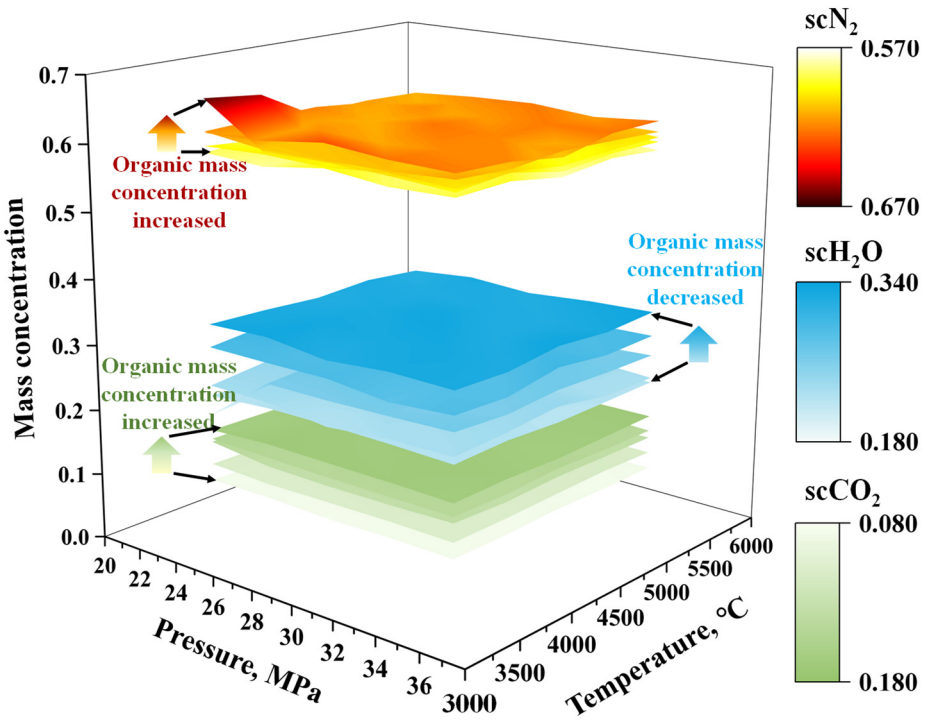


Figure 3. Change law of scMCTF composition.

This is because higher organic matter concentrations in the feedstock mean more organic content, leading to a higher total carbon count in the reaction system, which ultimately results in the formation of more $scCO_2$ after the reaction. At the same time, the more organic matter there is, the more feedwater is consumed in the reaction, so the concentration of scH_2O decreases as the organic matter concentration increases. Correspondingly, since the generation of $scCO_2$ and scH_2O consumes oxygen from the air, the more that is produced, the more oxygen is used. This means that the remaining nitrogen in the air, which does not participate in the reaction, increases, leading to a rise in scN_2 concentration with increasing organic matter concentration.

3.2. Change Law of Yield

Based on the scMCTF yield generated under different temperatures, pressures, and organic matter concentrations in the feedstock (Figure 4), it can be seen that higher pressure results in a higher thermal fluid yield, although this effect is relatively small. As the organic matter concentration in the feedstock increases, the yield decreases, while higher reaction temperatures lead to a higher yield, with temperature having a very significant impact on yield.

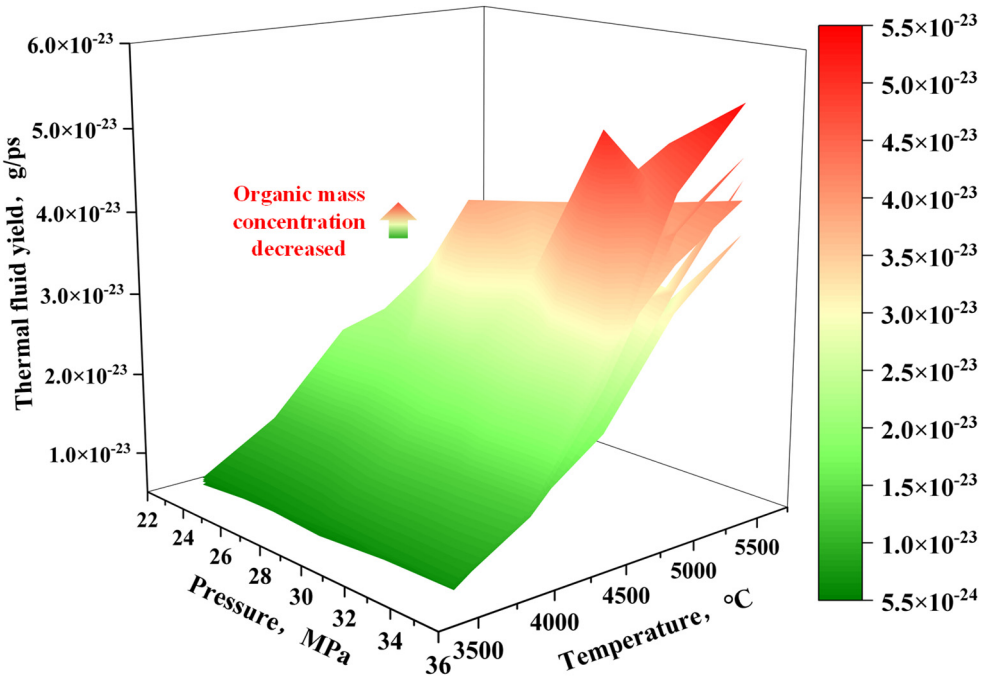


Figure 4. Change law of thermal fluids yield.

From the perspective of molecular collision theory, chemical reactions occur through collisions between molecules. The higher the pressure, the closer the initial distance between molecules, increasing the probability of collisions and thus raising the reaction yield as pressure increases. The effect of organic matter concentration on yield is relative. A higher organic matter concentration means more molecules per unit volume, which favors collisions and accelerates the reaction rate. However, the gasification reaction of organic matter in a supercritical water environment is sensitive to water concentration; the lower the water concentration and the higher the organic matter concentration, the less active the gasification reaction becomes [25]. As a result, the influence of organic matter concentration on yield is a combined effect of these two factors, with the latter being dominant. Higher temperatures increase molecular speed and kinetic energy, raising both collision energy and collision probability, thus enhancing the reaction rate and ultimately increasing the yield.

4. Model of scMCTF Composition and Yield Control

4.1. Model of Composition Control

Based on the previous analysis, it is evident that temperature and pressure have minimal impact on the composition of scMCTF. Therefore, their influence is neglected in the modeling process, and a correlation model is established between the scMCTF composition and the organic matter concentration in the feedstock. Additionally, since the sum of the three components in scMCTF equals 1, only the models for $scCO_2$ and scH_2O with respect to the organic matter concentration are developed.

As seen from the fitting results of $scCO_2$ and scH_2O with organic matter concentration (Figure 5), both $scCO_2$ and scH_2O follow a power function relationship with organic matter concentration, with the fitting coefficients of determination (R^2) exceeding 0.99, indicating

a high degree of fit. Therefore, an scMCTF composition control model can be established based on these fitting equations (Equations (1)–(3)), and the organic matter concentration required for the reaction can be calculated based on the desired content of a particular scMCTF component, thereby achieving control over the composition of scMCTF injected into the reservoir.

$$C(\mathrm{scH_2O}) = 0.1360C(\mathrm{OMC})^{-0.3582} \quad (1)$$

$$C(\mathrm{scCO_2}) = 0.3924C(\mathrm{OMC})^{0.6126} \quad (2)$$

$$C(\mathrm{scN_2}) = 1 - C(\mathrm{scH_2O}) - C(\mathrm{scCO_2}) \quad (3)$$

where $C(\mathrm{scH_2O})$, $C(\mathrm{scCO_2})$, and $C(\mathrm{scN_2})$ represent the mass concentrations of supercritical water, supercritical carbon dioxide, and supercritical nitrogen, respectively; f. OMC is the mass concentration of organic matter in the feedstock, f.

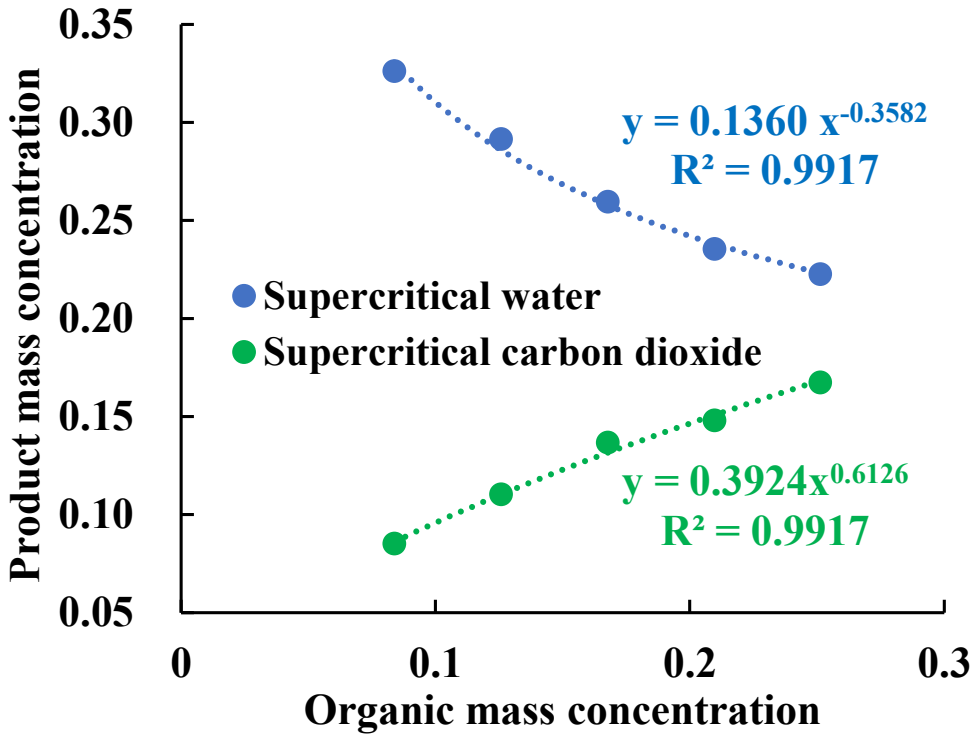


Figure 5. Relationship model between content and mass concentration.

4.2. Model of Yield Control

Compared to the composition control model, the yield control model is more complex because it is influenced by three factors: temperature, pressure, and organic matter concentration. Therefore, a control model is established based on a quadratic fitting approach. First, temperature and pressure are treated as independent variables, and a modified inverse linear logarithmic model is used to develop the relationship between temperature, pressure, and thermal fluid yield under different organic matter concentration conditions (Equation (4), Table 1). It is worth noting that 10^{-24} in Equation (4) is just an order of magnitude conversion coefficient of the fitting results and has no actual physical significance.

$$v = 10^{-24}\frac{TP}{a + b\ln(T)} \quad (4)$$

where v represents the molecular simulation thermal fluid yield, g·ps^{-1}. T is the reaction temperature, °C. P is the reaction pressure, and MPa. a and b are the model fitting coefficients, which are dimensionless.

Table 1. Model coefficients of different organic matter mass concentration conditions.

Number	Organic Mass Concentration, f	Fitting Coefficient *a*	Fitting Coefficient *b*	R^2
1	0.0839	1.11×10^5	-1.22×10^4	0.87
2	0.1259	1.08×10^5	-1.23×10^4	0.80
3	0.1679	1.37×10^5	-1.47×10^4	0.90
4	0.2097	1.37×10^5	-1.54×10^4	0.88
5	0.2514	1.57×10^5	-1.75×10^4	0.92

Based on the fitting coefficients *a*, *b*, and the corresponding organic matter concentration data, the relationship curves of fitting coefficient *a*—organic matter concentration and fitting coefficient *b*—organic matter concentration were plotted by Microsoft Office EXCEL 2019 (Figure 6). As shown in Figure 6, the fitting coefficient *a* increases as the feedstock organic matter concentration increases, while fitting coefficient *b* decreases with the increase of the feedstock organic matter concentration. The fitting equation for *a*, organic matter concentration, has a coefficient of determination R^2 of 0.88, and the fitting equation for *b*, organic matter concentration, has a coefficient of determination R^2 of 0.94. Both show a good linear relationship with the organic matter concentration. Therefore, the relationship models for fitting coefficient *a*, organic matter concentration, and fitting coefficient *b*, organic matter concentration, can be established (Equations (5) and (6)).

$$a = 2.90 \times 10^5 \mathrm{OMC} + 8.14 \times 10^4 \quad (5)$$

$$b = -3.27 \times 10^4 \mathrm{OMC} - 8.95 \times 10^3 \quad (6)$$

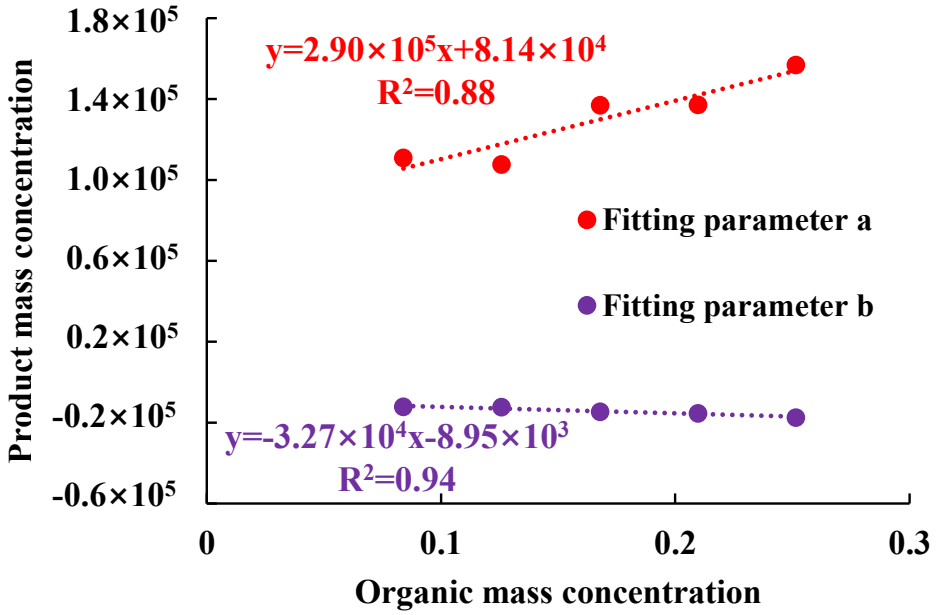


Figure 6. Relationship model between fitting coefficient and mass concentration.

By combining the temperature–pressure–thermal fluid yield correlation model (Equation (4)) with the fitting coefficient–organic matter concentration correlation models (Equations (5) and (6)), an organic matter concentration–temperature–pressure–thermal fluid yield correlation model is established, namely the scMCTF yield control model (Equation (7)). Using Equation (7), the scMCTF yield under specific temperature, pressure,

and feedstock organic matter concentration conditions can be calculated, thereby achieving the control of the scMCTF yield.

$$v = \frac{10^{-24}TP}{(2.90 \times 10^5 \mathrm{OMC} + 8.14 \times 10^4) - (3.27 \times 10^4 \mathrm{OMC} + 8.95 \times 10^3)\ln(T)} \quad (7)$$

5. Optimization Method of Synergistic scMCTF Composition and Yield

5.1. Conversion Relationship Between Yield and Injection Rate

In practical field applications, the injection rate of thermal fluids is typically above the ton/day scale [26], which is far greater than the scMCTF yield calculated using the reactive molecular dynamics model. This difference arises from the scale discrepancy between the thermal fluid generation systems. On-site systems are large-scale, meter-sized scMCTF generators, whereas the molecular model represents a nanoscale simulation box. Therefore, it is necessary to analyze the relationship between these two scenarios and establish a corresponding conversion model.

The scMCTF generation principle in large generators is consistent with the principle used in the molecular dynamic simulation model. Based on this, when the temperature and pressure inside the generator are the same as those inside the simulation box, the simulation box can be considered a microelement within the generator (Figure 7). This is because, under the same temperature and pressure conditions, substances share the same thermodynamic state.

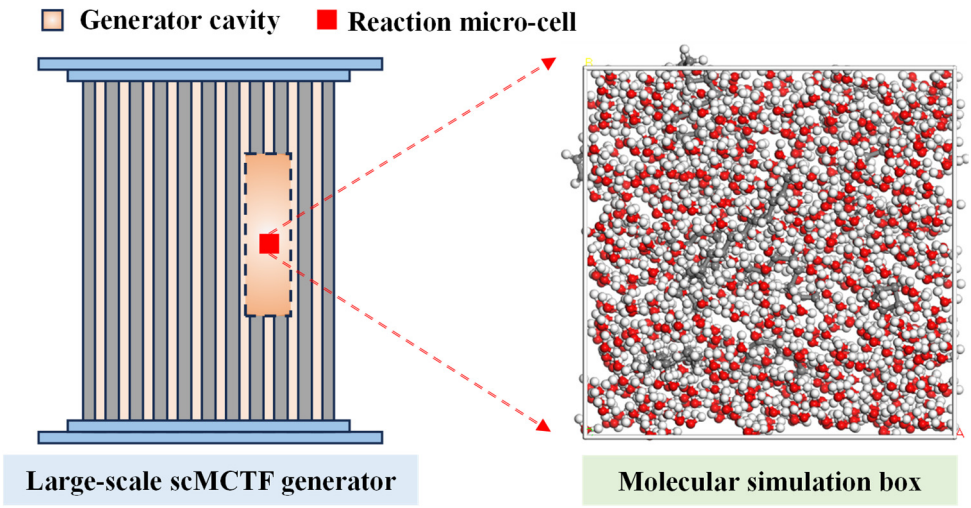


Figure 7. Comparison of scale relationship between scMCTF generator and molecular simulation box.

Therefore, the scMCTF generator in the field can be viewed as being composed of countless microelements or, in other words, countless simulation boxes. The conversion relationship between them depends on the number of microelements inside the generator. The scMCTF generation scale in the field is X times the scMCTF generation scale in the simulation box, where X is the ratio of the generator's internal volume to the simulation box volume. Under the same temperature and pressure conditions, the fluid density inside the generator and the simulation box is identical, meaning the volume ratio X equals the mass ratio Y of the fluid inside them. Furthermore, under the same organic matter concentration, the mass ratio of the fluid is effectively equal to the mass ratio of the organic matter, Z. For example, if the mass of organic matter in the simulation box is 1 g and the mass of organic matter in the field generator is 1000 g, the scMCTF injection rate in the field will be 1000 times the scMCTF yield in the simulation box. In the simulations mentioned earlier, the organic matter used was a mixture of five molecules of hexadecane (paraffin), three molecules of cyclopentane (naphthene), one molecule of benzene (monocyclic aromatic hydrocarbon), and one molecule of naphthalene (bicyclic aromatic hydrocarbon), with a total mass of 2.572×10^{-24} kg. Based

on this, a conversion relationship (Equation (8)) between the scMCTF yield and injection rate is established. Combining Equations (7) and (8), the scMCTF injection rate for offshore heavy oil development platforms under various reaction conditions can be calculated.

$$I = \frac{m}{2.572 \times 10^{-24}} v \tag{8}$$

where I represents the scMCTF injection rate for offshore heavy oil development platforms, g·ps^{-1}. m represents the mass of organic matter placed in the platform's scMCTF generator, kg.

5.2. Synergistic Optimization Method

As previously discussed, in field applications, the composition of the scMCTF injected into the heavy oil reservoir and the injection rate are two crucial parameters. These parameters are determined simultaneously at the scMCTF generation point on the platform and are not affected in subsequent flow stages. Therefore, it is essential to optimize both the composition and the injection rate in coordination.

Based on the established control models (Equations (1)–(3), (7) and (8)), the composition of scMCTF is primarily controlled by the organic matter concentration, while the injection rate of scMCTF is influenced by temperature, pressure, and organic matter concentration. Thus, a method for optimizing both the scMCTF composition and injection rate is proposed (Figure 8). First, determine the required organic matter concentration based on the target scMCTF composition. Then, based on the temperature and pressure tolerance limits of the platform's scMCTF generator, along with other technical and economic factors, define an acceptable range for reaction temperature and pressure. Within this range, select a specific temperature–pressure combination. Next, input the determined organic matter concentration and selected temperature–pressure data into the scMCTF yield control equation to calculate the corresponding yield under these conditions. Using the conversion relationship between the yield and injection rate, determine the scMCTF injection rate. Finally, assess whether the obtained injection rate meets the target. If it does, the optimization process ends; if not, adjust the temperature and pressure values and repeat the optimization process until the injection rate reaches the desired target.

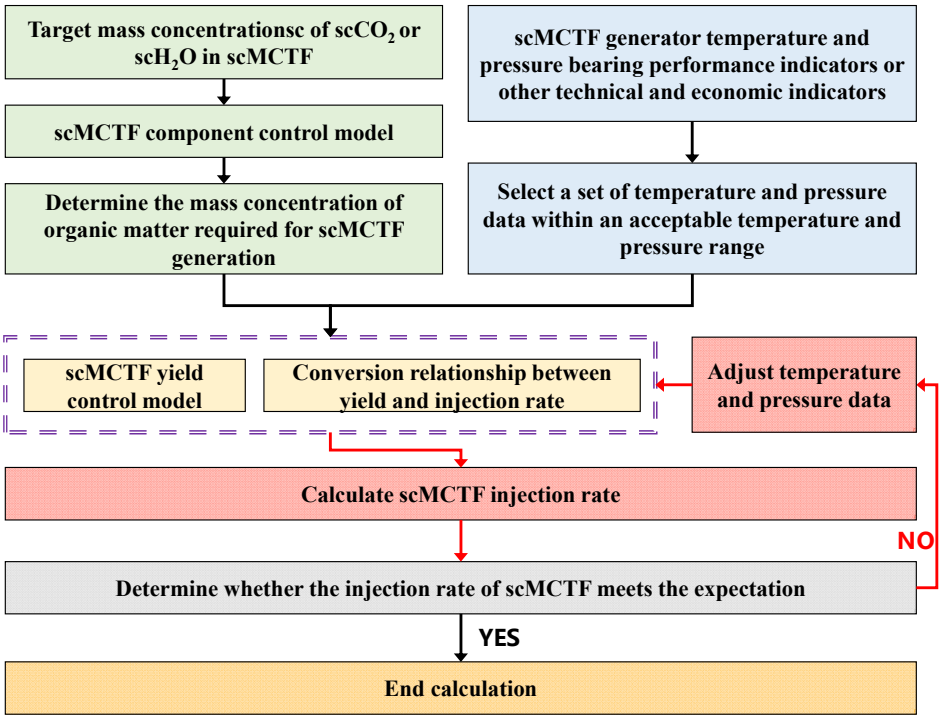


Figure 8. Work flow.

6. Discussion

Currently, laboratory studies on steam-assisted gravity drainage for heavy oil recovery using injected scMCTF rarely consider the impact of differences in fluid composition or injection rate on recovery efficiency [1–3,27]. However, optimizing the content of non-condensable gasses in the thermal fluid and the injection rate is critical for adjusting injection parameters to achieve the best thermal recovery results [28]. The newly proposed synergistic optimization method, based on the scMCTF composition and yield control model, offers a novel global optimization approach. It enables the simultaneous calculation of optimal reaction conditions required to achieve the desired scMCTF composition and injection rate while considering technical, economic, and equipment limitations on-site, thereby significantly enhancing injection operation efficiency.

Despite its advantages, the proposed method also has some limitations, which include the following two points:

(1) Inability to independently control $scCO_2$ and scN_2 content. Since the control equations for scH_2O (Equation (1)) and $scCO_2$ (Equation (2)) are both primarily influenced by organic matter concentration, once one of these components is determined, the other is passively fixed. According to the relationship between $scCO_2$, scH_2O, and scN_2 (Equation (3)), once the $scCO_2$ and scH_2O contents are determined, the scN_2 content is also fixed. In other words, the control equations can only adjust the content of one of the non-condensable gasses, whereas current research often aims to determine the ratio of these two gasses [28].

(2) Limited consideration of influencing factors. The current experiments, simulations, and models focus only on the three most fundamental factors: temperature, pressure, and organic matter concentration. However, other factors also affect the reaction, such as the type of feedstock [29,30], reaction time [31,32], catalyst type, and concentration [33,34]. Expanding the range of influencing factors would enhance the adaptability of the optimization method, enabling its application to a broader set of field conditions and unlocking more opportunities for technical parameter optimization in the field, thereby improving the efficiency of scMCTF thermal recovery operations.

Given these limitations, future research should focus on the following key areas:

(1) Improving the quality of control equations to enable independent control of individual component concentrations.

(2) Developing control equations that incorporate additional factors based on field requirements, enhancing the versatility of the optimization method. This would expand its application scope and provide more flexibility for field parameter adjustments, leading to more efficient scMCTF thermal recovery operations.

7. Conclusions

(1) The influence of temperature and pressure on the composition of supercritical multicomponent thermal fluid (scMCTF) is not significant, while the composition is largely influenced by the organic matter concentration in the feedstock. As the organic matter concentration increases, the content of supercritical carbon dioxide ($scCO_2$) and supercritical nitrogen (scN_2) rises, while the content of supercritical water (scH_2O) decreases.

(2) Temperature, pressure, and the organic matter concentration in the feedstock all have an impact on the scMCTF yield. Higher temperatures and pressures lead to a higher scMCTF yield, while a higher organic matter concentration results in a lower yield.

(3) Using data fitting methods, control models for scMCTF composition and yield were developed. The scMCTF composition fitting model follows a power function relationship, with a coefficient of determination (R^2) greater than 0.9. The scMCTF yield fitting model follows a modified inverse linear logarithmic function, with an R^2 greater than 0.8, indicating a high degree of fit for both the composition and yield control models.

(4) The ratio between scMCTF production in molecular simulations and the actual scMCTF injection rate in the field is proportional to the ratio of the mass of organic matter in the platform's scMCTF generator to that in the simulation box. This allows for the conversion of scMCTF yields from simulation-scale to actual field-scale injection rates.
(5) Based on the established composition and yield control models, along with the proposed conversion relationship between the scMCTF yield and injection rate, a synergistic optimization method for scMCTF composition and the injection rate was developed. This provides an effective technical approach for simultaneously adjusting and optimizing scMCTF composition and the injection rate in field operations.

Author Contributions: Methodology, M.D. and W.Y.; Investigation, J.T.; Writing—original draft, S.Y.; Writing—review & editing, W.Z.; Supervision, Z.Q. and W.Y. All authors have read and agreed to the published version of the manuscript.

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Data Availability Statement: The data presented in this study are available on request from the corresponding author. The data are not publicly available due to privacy restrictions.

Conflicts of Interest: The authors declare no conflict of interest.

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