Claims

1. An optimization method for a whole process of molecular-level oil refinery processing, wherein the optimization method comprising:

acquiring molecular composition of crude oil;

acquiring molecular composition of various fractions obtained by distillation of the crude oil according to physical properties of various single molecules in the molecular composition of the crude oil;

respectively inputting, according to a preset feedstock ratio, the corresponding fractions into a product prediction model of a respective petroleum processing device as petroleum processing feedstocks, to obtain molecular composition of a corresponding predicted product and content of each single molecule in the predicted product;

blending each of the predicted products which is used as a product blending feedstock according to a preset rule set, to obtain molecular composition of a plurality of mixed products and content of each single molecule in each of the mixed products;

respectively calculating a product property of each of the mixed products according to the molecular composition of each of the mixed products and the content of each single molecule in each of the mixed products; and determining whether the product property of each of the mixed products meets any preset standard in a preset standard set;

if the product property of each of the mixed products meets any preset standard in the preset standard set, acquiring a target parameter according to all mixed products and determining whether the target parameter meets a preset condition; and

if the target parameter does not meet the preset condition, adjusting the preset feedstock ratio, a parameter in the product prediction model and a preset rule in the preset rule set, to re-obtain a plurality of mixed products until the product property of each of the mixed products meets any preset standard in the preset standard set and the target parameter meets the preset condition.

2. The optimization method according to claim 1, wherein the optimization method further comprises:

acquiring an input flow of petroleum processing feedstocks input to each of the petroleum processing devices;

determining whether each of the input flows meets a preset input flow range of the respective petroleum processing device; and

adjusting the preset feedstock ratio if any one of the input flows does not meet the preset input flow range of the respective petroleum processing device, and respectively re-inputting, according to the adjusted preset feedstock ratio, the corresponding fractions into the product prediction model of the respective petroleum processing device as petroleum processing feedstocks, until each of the input flows meets the preset input flow range of the respective petroleum processing device.

3. The optimization method according to claim 1, wherein the optimization method further comprises:

acquiring molecular composition of the petroleum processing feedstocks inputted to each of the petroleum processing devices and content of each single molecule in the petroleum processing feedstocks;

calculating a physical property of each single molecule in the petroleum processing feedstocks, calculating a feedstock property of the petroleum processing feedstocks according to the physical property of each single molecule and the content of each single molecule in the petroleum processing feedstocks;

determining whether each of the feedstock properties meets a preset physical property restriction interval of the respective petroleum processing device; and

if any of the feedstock properties does not meet the preset physical property restriction interval of the respective petroleum processing device, adjusting the preset feedstock ratio, and respectively re-inputting, according to the adjusted preset feedstock ratio, the corresponding fractions into the product prediction model of the respective petroleum processing device as petroleum processing feedstocks, until each of the feedstock properties meets the preset physical property restriction interval of the respective petroleum processing device.

4. The optimization method according to claim 1, wherein the acquiring a target parameter according to all mixed products and determining whether the target parameter meets a preset condition comprises:

acquiring a product price of each of mixed products and a yield of each of mixed products;

calculating a product benefit of each of mixed products according to the yield of each of mixed products and the product price of each of mixed products;

accumulating the product benefit of each of mixed products to obtain a cumulative benefit;

acquiring a feedstock price of each group of the petroleum processing feedstocks and an operating cost of each of the petroleum processing devices;

subtracting feedstock prices of all petroleum processing feedstocks and operating costs of all petroleum processing devices from the cumulative benefit to obtain a comprehensive benefit;

serving the comprehensive benefit as the target parameter;

determining whether the comprehensive benefit reaches a maximum value;

determining that the target parameter meets the preset condition if the comprehensive benefit reaches the maximum value; and

determining that the target parameter does not meet the preset condition if the comprehensive benefit does not reach the maximum value.

5. The optimization method according to claim 1, wherein the optimization method further comprises:

if the product property of any mixed product does not meet any preset standard in the preset standard set, adjusting the preset rule in the preset rule set and blending each of the product blending feedstocks according to the adjusted preset rule set, to re-obtain a plurality of mixed products until the product property of each of the mixed products meets any preset standard in the preset standard set.

6. The optimization method according to claim 1, wherein the respectively calculating a product property of each of the mixed products according to the molecular composition of each of the mixed products and the content of each single molecule in each of the mixed products comprises:

acquiring first molecular composition of each group of the product blending feedstocks and first component content of each single molecule in each group of the product blending feedstocks;

based on the preset rule set, obtaining second molecular composition of each of mixed products and second component content of each single molecule in each of mixed products according to the first molecular composition of each group of the product blending feedstock and the first component content of each single molecule in each group of the product blending feedstocks;

calculating a physical property of each single molecule in each of the mixed products according to the number of groups of each group contained in each single molecule in each of the mixed products and a contribution value of each group to the physical property; and

calculating a product property of each of the mixed products according to the physical property and the second component content of each single molecule in each of the mixed products.

7. The optimization method according to claim 6, wherein calculation of the physical property of each single molecule comprises:

for each single molecule, acquiring the number of groups of each group constituting the single molecule and a contribution value of each group to the physical property; and

inputting the number of groups of each group constituting the single molecule and the contribution value of each group to the physical property into a pre-trained property calculation model, to acquire the physical property of the single molecule outputted by the pre-trained property calculation model.

8. The optimization method according to claim 7, wherein, before the inputting the number of groups of each group constituting the single molecule and the contribution value of each group to the physical property into a pre-trained property calculation model, the optimization method further comprises:

comparing the number of groups of each group constituting the single molecule with molecular information of a template single molecule with known physical properties pre-stored in a database, the molecular information comprising the number of groups of each group constituting the template single molecule;

determining whether there is a same template single molecule as the single molecule;

if there is a same template single molecule as the single molecule, outputting the physical properties of the template single molecule as a physical property of the single molecule; and

if there is not a same template single molecule as the single molecule, then performing the step of the inputting the number of groups of each group constituting the single molecule and the contribution value of each group to the physical property into a pre-trained property calculation model.

9. The optimization method according to claim 1, wherein the acquiring molecular composition of various fractions obtained by distillation of the crude oil according to

physical properties of various single molecules in the molecular composition of the crude oil comprises:

acquiring each single molecule in the crude oil and the content of each single molecule;

calculating a boiling point of each single molecule, respectively; and

cutting the crude oil by distillation according to a preset fractional distillation range to obtain multiple fractions, and determining a single molecule and content of each single molecule contained in each of the fractions according to the boiling point and the content of each single molecule in the crude oil.

10. The optimization method according to claim 9, wherein the optimization method further comprises:

for two fractions with adjacent distillation ranges, taking the fraction with a relatively high temperature in the distillation range as a first fraction, and taking the fraction with a relatively low temperature in the distillation range as a second fraction;

calculating a minimum value of an overlapping interval of an overlapping distillation range of the first fraction and the second fraction by the following formula:

$T_{\min} = T_{\text{cut}} \times (1 - SF)$; and

calculating a maximum value of the overlapping interval of the overlapping distillation range of the first fraction and the second fraction by the following formula:

$T_{\max} = T_{\text{cut}} \times (1 + SF)$;

where, $T_{\min}$ is the minimum value of the overlapping interval, $T_{\max}$ is the maximum value of the overlapping interval, T_{cut} is the distillation cut temperature of the first fraction and the second fraction, and SF is a separation index of the first fraction and the second fraction.

11. The optimization method according to claim 10, wherein the optimization method further comprises:

calculating content of distilled part into the first fraction of each single molecule in the overlapping interval and calculating content of distilled part into the second frac tion of each single molecule in the overlapping interval according to the content of

each single molecule and each single molecule corresponding to each boiling point of the overlapping interval;

wherein the content of distilled part into the first fraction of each single molecule in the overlapping interval and the content of distilled part into the second fraction of each single molecule in the overlapping interval are calculated by the following equation:

$$C_h^i = \ln\left(\frac{T_i}{T_{\min}}\right) \times C^i;$$

$$C_l^i = C^i - C_h^i;$$

where, C_h^i is the content of distilled part into the first fraction of the i-th single molecule in all molecules with a boiling point located in the overlapping interval, which the i-th single molecule has the boiling point located in the overlapping interval, C_l^i is the content of distilled part into the first fraction of the i-th single molecule in all molecules with a boiling point located in the overlapping interval, which the i-th single molecule has the boiling point located in the overlapping interval, T_i is the boiling point of the i-th single molecule, $T_{\min}$ is the minimum value of the overlapping interval, and C^i is the content of the i-th single molecule in all molecules with a boiling point located in the overlapping interval, which the i-th single molecule has the boiling point located in the overlapping interval; and

obtaining the content of each single molecule and each single molecule in each of the first fraction and the second fraction after the crude oil is cut by distillation according to the content of distilled part into the first fraction of each single molecule in the overlapping interval and the content of distilled part into the second fraction of each single molecule in the overlapping interval.

12. The optimization method according to claim 9, wherein the calculating a boiling point of each single molecule comprises:

for each of the single molecule, acquiring the number of groups of each group constituting the single molecule and a contribution value of each group to the boiling point; and

inputting the number of groups of each group constituting the single molecule and the contribution value of each group to the boiling point into a pre-trained property calculation

model, to acquire the boiling point of the single molecule outputted by the pre-trained property calculation model.

13. The optimization method according to claim 12, wherein, before the inputting the number of groups of each group constituting the single molecule and the contribution value of each group to the boiling point into a pre-trained property calculation model, the optimization method further comprises:

comparing the number of groups of each group constituting the single molecule with molecular information of a template single molecule with known boiling point pre-stored in a database, the molecular information comprising the number of groups of each group constituting the template single molecule;

determining whether there is a same template single molecule as the single molecule;

if there is a same template single molecule as the single molecule, outputting the boiling point of the template single molecule as a boiling point of the single molecule; and

if there is not a same template single molecule as the single molecule, then performing the step of the inputting the number of groups of each group constituting the single molecule and the contribution value of each group to the boiling point into a pre-trained property calculation model.

14. The optimization method according to claim 7 or 12, wherein a step of training the property calculation model comprises:

constructing a property calculation model of a single molecule;

acquiring the number of groups of each group constituting a sample single molecule; wherein the physical property of the sample single molecule is known;

inputting the number of groups of each group constituting the sample single molecule into the property calculation model;

acquiring a predicted physical property of the sample single molecule outputted by the property calculation model;

if a deviation value between the predicted physical property and the physical property which is known is less than a preset deviation threshold, determining that the property calculation model converges, acquiring a contribution value corresponding to each group in the property calculation model which is converged, and storing the contribution value as a contribution value of the group to the physical property; and

if the deviation value between the predicted physical property and the physical property which is known is greater than or equal to the deviation threshold, adjusting a contribution value corresponding to each group in the property calculation model until the property calculation model converges.

15. The optimization method according to claim 14, wherein the property calculation model is established as shown below:

$$f = a + \sum_i n_i \Delta f_i ;$$

where, f is the physical property of the single molecule, n_i is the number of groups of the i-th group, Δf_i is the contribution value of the i-th group to the physical property, and a is an associated constant.

16. The optimization method according to claim 14, wherein the acquiring the number of groups of each group constituting a sample single molecule comprises:

determining a primary group, the number of groups of the primary group, a multi-stage group, and the number of groups of the multi-stage group in all groups of the single molecule;

taking all groups constituting the single molecule as the primary group; and

taking various groups which coexist and contribute to a same physical property in common as the multi-stage group, and taking the number of the various groups as a level of the multi-stage group.

17. The optimization method according to claim 16, wherein,

the property calculation model is established as shown below:

$$f = a + \sum_i \mathrm{m}_{1i} \Delta f_{1i} + \sum_j m_{2j} \Delta f_{2j} ..... + \sum_l m_{Nl} \Delta f_{Nl} ;$$

where, f is the physical property of the single molecule, m_{1i} is the number of groups of the i-th group in the primary group, Δf_{1i} is the contribution value of the i-th group in the primary group to the physical property, m_{2j} is the number of groups of the j-th group in a secondary group, Δf_{2j} is the contribution value of the j-th group in the secondary group to the physical property, m_{Nl} is the number of groups of the l-th group in an N-stage

group, Δf_{Nl} is the contribution value of the l-th group in the N-stage group to the physical property, a is an associated constant, and *N* is a positive integer greater than or equal to 2.

18. The optimization method according to claim 12, wherein the acquiring the number of groups of each group constituting the single molecule comprises:

determining a primary group, the number of groups of the primary group, a multi-stage group, and the number of groups of the multi-stage group in all groups of the single molecule;

taking all groups constituting the single molecule as the primary group; and

taking various groups which coexist and contribute to a same physical property in common as the multi-stage group, and taking the number of the various groups as a level of the multi-stage group.

19. The optimization method according to claim 18, wherein,

the inputting the number of groups of each group constituting the single molecule and the contribution value of each group to the boiling point~~physical property~~ into a pre-trained property calculation model, to acquire the boiling point of the single molecule outputted by the pre-trained property calculation model comprises:

calculating the boiling point of the single molecule according to the following the property calculation model:

$$T = \frac{SOL \times GROUP_1 + SOL \times GROUP_2 + ... + SOL \times GROUP_{\mathrm{N}}}{(SOL \times N\mathrm{umh})^d + b} + c;$$

where, T is the boiling point of the single molecule, SOL is a single molecule vector converted according to the number of groups of each group constituting the single molecule, $GROUP_{11}$ is a first contribution value vector converted according to a contribution value of the primary group to the boiling point, $GROUP_{12}$ is a second contribution value vector converted according to a contribution value of the secondary group to the boiling point, $GROUP_{1\mathrm{N}}$ is an N-th contribution value vector converted according to a contribution value of the N-stage group to the boiling point, $N\mathrm{umh}$ is the number of atoms other than the hydrogen atom in the single molecule, d is a first

preset constant, b is a second preset constant, c is a third preset constant, and N is a positive integer greater than or equal to 2.

20. The optimization method according to claim 19, wherein,

converting the single molecule vector according to the number of groups of each group constituting the single molecule comprises:

taking the number of species of groups as a dimension of the single molecule vector; and

taking the number of groups of each group as an element value of the corresponding dimension in the single molecule vector,

converting the first contribution value vector according to a contribution value of the primary group to the boiling point comprises:

taking the number of types of primary groups as a dimension of the first contribution value vector; and

taking the contribution value of each primary group to the boiling point as an element value of the corresponding dimension in the first contribution value vector,

converting the second contribution value vector according to a contribution value of the secondary group to the boiling point comprises:

taking the number of types of secondary groups as a dimension of the second contribution value vector; and

taking the contribution value of each secondary group to the boiling point as an element value of the corresponding dimension in the second contribution value vector,

converting the N-th contribution value vector according to a contribution value of each N-stage group to the boiling point comprises:

taking the number of types of N-stage groups as a dimension of the N-th contribution value vector; and

taking the contribution value of each N-stage group to the boiling point as an element value of the corresponding dimension in the N-th contribution value vector.

21. The optimization method according to claim 1, wherein the respectively inputting, according to a preset feedstock ratio, the corresponding fractions into a product prediction model of a respective petroleum processing device comprises:

obtaining different amounts of each fraction according to the preset feedstock ratio, and respectively inputting each fraction into the product prediction model of the respective petroleum processing device,

the petroleum processing device comprises a catalytic cracking unit, a delayed coking unit, a residue hydrotreating unit, a hydrocracking unit, a diesel hydro-upgrading unit, a diesel hydro-refining unit, a gasoline hydro-refining unit, a catalytic reforming unit and an alkylation unit.

22. The optimization method according to claim 21, wherein, a step of training the product prediction model comprises:

establishing a product prediction model; wherein the product prediction model comprises: a set of reaction rules comprising a plurality of reaction rules and a reaction rate algorithm;

acquiring sample feedstock information for a sample feedstock;

training the set of reaction rules by using the sample feedstock information, and fixing the set of reaction rules that has been trained; and

training the reaction rate algorithm by using the sample feedstock information, and fixing the reaction rate algorithm that has been trained, to obtain the product prediction model that has been trained.

23. The optimization method according to claim 22, wherein the sample feedstock information of the sample feedstock comprises: molecular composition of the sample feedstock, molecular content of each molecule in the sample feedstock, molecular composition of an actual product corresponding to the sample feedstock, and actual content of each molecule in the actual product.

24. The optimization method according to claim 23, wherein the training the set of reaction rules by using the sample feedstock information comprises:

processing the molecular composition of the sample feedstock according to a preset set of reaction rules, to obtain a reaction pathway corresponding to each molecule in the molecular composition of the sample feedstock;

obtaining first molecule composition of a device output product comprising the sample feedstock, an intermediate product, and a predicted product according to the reaction path corresponding to each molecule in the molecular composition of the sample feedstock; in the device output product, comprising: the sample feedstock, the intermediate product, and the predicted product;

calculating a first relative deviation according to the first molecular composition of the device output product and second molecular composition of the actual product;

if the first relative deviation meets a preset condition, fixing the set of reaction rules; and

if the first relative deviation does not meet the preset condition, adjusting a reaction rule in the set of reaction rules, and recalculating the first relative deviation according to the adjusted set of reaction rules until the first relative deviation meets the preset condition.

25. The optimization method according to claim 24, wherein the calculating a first relative deviation according to the first molecular composition of the device output product and second molecular composition of the actual product comprises:

acquiring species of single molecules in the first molecule composition, to constitute a first set;

acquiring species of single molecules in the second molecule composition, to constitute a second set;

determining whether the second set is a subset of the first set;

if the second set is not a subset of the first set, obtaining a pre-stored relative deviation value that does not meet the preset condition as the first relative deviation; and

if the second set is a subset of the first set, calculating the first relative deviation by a calculating formula as follows:

$$x_1 = \frac{\text{card}\left((M - M_1 - M_2) - M_3\right)}{\text{card}\ (M - M_1 - M_2)}\ ;$$

where, x_1 is the first relative deviation, M is the first set, M_1 is a set of species of single molecules in the molecular composition of the sample feedstock, M_2 is a set of species of single molecules in the molecular composition of the intermediate product, M_3 is the second set, and card represents the number of elements in the sets.

26. The optimization method according to claim 23, wherein the training the reaction rate algorithm by using the sample feedstock information comprises:

calculating a reaction rate of a reaction path corresponding to each molecule in the molecular composition of the sample feedstock, respectively, according to the reaction rate algorithm;

obtaining predicted content of each molecule in a predicted product corresponding to the sample feedstock according to molecular content of each molecule in the sample feedstock and the reaction rate of the reaction path corresponding to the molecule;

calculating a second relative deviation according to the predicted content of each molecule in the predicted product and the actual content of each molecule in the actual product;

if the second relative deviation meets a preset condition, fixing the reaction rate algorithm; and

if the second relative deviation does not meet the preset condition, adjusting a parameter in the reaction rate algorithm, and recalculating the second relative deviation according to the adjusted reaction rate algorithm until the second relative deviation meets the preset condition.

27. The optimization method according to claim 26, wherein the calculating a reaction rate of a reaction path corresponding to each molecule in the molecular composition of the sample feedstock, respectively, according to the reaction rate algorithm comprises:

calculating a reaction rate of each reaction path according to a reaction rate constant in the reaction rate algorithm;

wherein the reaction rate constant is determined according to a calculation formula as follows:

$$k = \frac{k_B E}{h} \exp(\frac{E\Delta S - \Delta E}{RE}) \varphi \times P^{\alpha} ;$$

where, k is the reaction rate constant, k_B is the Boltzmann constant, h is the Planck constant, R is an ideal gas constant, E is a temperature value of the environment at which the reaction path is located, $\exp$ is an exponential function with base of natural constant, ΔS is an entropy change before and after the reaction corresponding to the reaction rule corresponding to the reaction path, ΔE is a reaction energy barrier corresponding to the reaction rule corresponding to the reaction path, φ is a catalyst activity factor, P is a pressure value of the environment at which the reaction path is located, and α is a pressure influencing factor corresponding to the reaction rule corresponding to the reaction path.

28. The optimization method according to any one of claims 21-27, wherein each petroleum processing device corresponds to a set of reaction rules.

29. An optimization apparatus for a whole process of molecular-level oil refinery and processing, wherein the optimization apparatus comprising:

an acquisition unit configured to acquire molecular composition of crude oil;

a first processing unit configured to acquire molecular composition of various fractions obtained by distillation of the crude oil according to physical properties of various single molecules in the molecular composition of the crude oil, and respectively input, according to a preset feedstock ratio, the corresponding fractions into a product prediction model of a respective petroleum processing device as petroleum processing feedstocks, to obtain molecular composition of a corresponding predicted product and content of each single molecule in the predicted product;

a second processing unit configured to blend each of the predicted products which is used as a product blending feedstock according to a preset rule set, to obtain molecular composition of a plurality of mixed products and content of each single molecule in each of the mixed products;

a third processing unit configured to respectively calculate a product property of each of the mixed products according to the molecular composition of each of the mixed products and the content of each single molecule in each of the mixed products; and determine whether the product property of each of the mixed products meets any preset standard in a preset standard set; and

a fourth processing unit configured to, if the product property of each of the mixed products meets any preset standard in the preset standard set, acquire a target parameter according to all mixed products and determine whether the target parameter meets a preset condition, and, if the target parameter does not meet the preset condition, adjust the preset feedstock ratio, a parameter in the product prediction model and a preset rule in the preset rule set, to re-obtain a plurality of mixed products until the product property of each of the mixed products meets any preset standard in the preset standard set and the target parameter meets the preset condition.

30. The optimization apparatus according to claim 29, wherein the optimization apparatus further comprises:

a flow control unit configured to acquire an input flow of petroleum processing feedstocks input to each of the petroleum processing devices, determine whether each of the input flows meets a preset input flow range of the respective petroleum processing device; and adjust the preset feedstock ratio if any one of the input flows does not meet the preset input flow range of the respective petroleum processing device, and respectively re-input, according to the adjusted preset feedstock ratio, the corresponding fractions into the

product prediction model of the respective petroleum processing device as petroleum processing feedstocks, until each of the input flows meets the preset input flow range of the respective petroleum processing device.

31. The optimization apparatus according to claim 29, wherein the optimization apparatus further comprises:

an in-feed property control unit configured to acquire molecular composition of the petroleum processing feedstocks inputted to each of the petroleum processing devices and content of each single molecule in the petroleum processing feedstocks, calculate a physical property of each single molecule in the petroleum processing feedstocks, calculate a feedstock property of the petroleum processing feedstocks according to the physical property of each single molecule and the content of each single molecule in the petroleum processing feedstocks, determine whether each of the feedstock properties meets a preset physical property restriction interval of the respective petroleum processing device; and, if any of the feedstock properties does not meet the preset physical property restriction interval of the respective petroleum processing device, adjust the preset feedstock ratio and respectively re-input, according to the adjusted preset feedstock ratio, the corresponding fractions into the product prediction model of the respective petroleum processing device as petroleum processing feedstocks, until each of the feedstock properties meets the preset physical property restriction interval of the respective petroleum processing device.

32. The optimization apparatus according to claim 29, wherein the fourth processing unit is, in particular, configured to acquire a product price of each of mixed products and a yield of each of mixed products, calculate a product benefit of each of mixed products according to the yield of each of mixed products and the product price of each of mixed products, accumulate the product benefit of each of mixed products to obtain a cumulative benefit, acquire a feedstock price of each group of the petroleum processing feedstocks and an operating cost of each of the petroleum processing devices, subtract feedstock prices of all petroleum processing feedstocks and operating costs of all petroleum processing devices from the cumulative benefit to obtain a comprehensive benefit, serve the comprehensive benefit as the target parameter, determine whether the comprehensive benefit reaches a maximum value, determine that the target parameter meets the preset condition if the comprehensive benefit reaches the maximum value; and determine that the target parameter does not

meet the preset condition if the comprehensive benefit does not reach the maximum value.

33. The optimization apparatus according to claim 29, wherein the optimization apparatus further comprises:

a product property control unit configured to, if the product property of any mixed product does not meet any preset standard in the preset standard set, adjust the preset rule in the preset rule set and blend each of the product blending feedstocks according to the adjusted preset rule set, to re-obtain a plurality of mixed products until the product property of each of the mixed products meets any preset standard in the preset standard set.

34. The optimization apparatus according to claim 29, wherein the third processing unit is, in particular, configured to acquire first molecular composition of each group of the product blending feedstocks and first component content of each single molecule in each group of the product blending feedstocks, based on the preset rule set, obtain second molecular composition of each of mixed products and second component content of each single molecule in each of mixed products according to the first molecular composition of each group of the product blending feedstock and the first component content of each single molecule in each group of the product blending feedstocks, calculate a physical property of each single molecule in each of the mixed products according to the number of groups of each group contained in each single molecule in each of the mixed products and a contribution value of each group to the physical property; and calculate a product property of each of the mixed products according to the physical property and the second component content of each single molecule in each of the mixed products.

35. The optimization apparatus according to claim 34, wherein the third processing unit is, in particular, configured to, for each single molecule, acquire the number of groups of each group constituting the single molecule and a contribution value of each group to the physical property; and input the number of groups of each group constituting the single molecule and the contribution value of each group to the physical property into a pre-trained property calculation model, to acquire the physical property of the single molecule outputted by the pre-trained property calculation model.

36. The optimization apparatus according to claim 35, wherein the optimization apparatus further comprises:

a single molecule property template matching unit configured to compare the number of groups of each group constituting the single molecule with molecular information of a template single molecule with known physical properties pre-stored in a database, the

molecular information comprising the number of groups of each group constituting the template single molecule, determine whether there is a same template single molecule as the single molecule, if there is a same template single molecule as the single molecule, output the physical properties of the template single molecule as a physical property of the single molecule; and if there is not a same template single molecule as the single molecule, then perform, by the third processing unit, the step of the inputting the number of groups of each group constituting the single molecule and the contribution value of each group to the physical property into a pre-trained property calculation model.

37. The optimization apparatus according to claim 29, wherein the first processing unit is, in particular, configured to acquire each single molecule in the crude oil and the content of each single molecule, calculate a boiling point of each single molecule, respectively, cut the crude oil by distillation according to a preset fractional distillation range to obtain multiple fractions, and determine a single molecule and content of the single molecule contained in each of the fractions according to the boiling point and the content of each single molecule in the crude oil.

38. The optimization apparatus according to claim 37, wherein the first processing unit is further configured to, for two fractions with adjacent distillation ranges, take the fraction with a relatively high temperature in the distillation range as a first fraction, and take the fraction with a relatively low temperature in the distillation range as a second fraction;

calculate a minimum value of an overlapping interval of an overlapping distillation range of the first fraction and the second fraction by the following formula:

$T_{\min} = T_{\text{cut}} \times (1 - SF)$; and

calculate a maximum value of the overlapping interval of the overlapping distillation range of the first fraction and the second fraction by the following formula:

$T_{\max} = T_{\text{cut}} \times (1 + SF)$;

where, $T_{\min}$ is the minimum value of the overlapping interval, $T_{\max}$ is the maximum value of the overlapping interval, T_{cut} is the distillation cut temperature of

the first fraction and the second fraction, and SF is a separation index of the first fraction and the second fraction.

39. The optimization apparatus according to claim 38, wherein the first processing unit is further configured to calculate content of distilled part into the first fraction of each single molecule in the overlapping int erval and calculate content of distilled part into the second fraction of each single molecule in the overlapping interval according to the content of each single molecule and each single molecule corresponding to each boiling point of the overlapping interval, and obtain the content of each single molecule and each single molecule in each of the first fraction and the second fraction after the crude oil is cut by distillation according to the content of distilled part into the first fraction of each single molecule in the overlapping interval and the content of distilled part into the second fraction of each single molecule in the overlapping interval,

wherein the content of distilled part into the first fraction of each single molecule in the overlapping interval and the content of distilled part into the second fraction of each single molecule in the overlapping interval are calculated by the following equation:

$$C_h^i = \ln\left(\frac{T_i}{T_{\min}}\right) \times C^i;$$

$$C_l^i = C^i - C_h^i;$$

where, C_h^i is the content of distilled part into the first fraction of the i-th single molecule in all molecules with a boiling point located in the overlapping interval, which the i-th single molecule has the boiling point located in the overlapping interval, C_l^i is the content of distilled part into the first fraction of the i-th single molecule in all molecules with a boiling point located in the overlapping interval, which the i-th single molecule has the boiling point located in the overlapping interval, T_i is the boiling point of the i-th single molecule, $T_{\min}$ is the minimum value of the overlapping interval, and C^i is the content of the i-th single molecule in all molecules with a boiling point located in the overlapping interval, which the i-th single molecule has the boiling point located in the overlapping interval.

40. The optimization apparatus according to claim 37, wherein the first processing unit is, in particular, configured to, for each of the single molecule, acquire the number of

groups of each group constituting the single molecule and a contribution value of each group to the boiling point; and input the number of groups of each group constituting the single molecule and the contribution value of each group to the boiling point into a pre-trained property calculation model, to acquire the boiling point of the single molecule outputted by the pre-trained property calculation model.

41. The optimization apparatus according to claim 40, wherein the optimization apparatus further comprises:

a single-molecule boiling point template matching unit configured to compare the number of groups of each group constituting the single molecule with molecular information of a template single molecule with known boiling point pre-stored in a database, the molecular information comprising the number of groups of each group constituting the template single molecule, determine whether there is a same template single molecule as the single molecule, if there is a same template single molecule as the single molecule, output the boiling point of the template single molecule as a boiling point of the single molecule; and if there is not a same template single molecule as the single molecule, then perform, by the first processing unit, the step of the inputting the number of groups of each group constituting the single molecule and the contribution value of each group to the boiling point into a pre-trained property calculation model.

42. The optimization apparatus according to claim 35, wherein the optimization apparatus further comprises:

a model training unit configured to construct a property calculation model of a single molecule, acquire the number of groups of each group constituting a sample single molecule; wherein the physical property of the sample single molecule is known, input the number of groups of each group constituting the sample single molecule into the property calculation model, acquire a predicted physical property of the sample single molecule outputted by the property calculation model, if a deviation value between the predicted physical property and the physical property which is known is less than a preset deviation threshold, determine that the property calculation model converges, acquire a contribution value corresponding to each group in the property calculation model which is converged, and store the contribution value as a contribution value of the group to the physical property; and, if the deviation value between the predicted physical property and the physical property

which is known is greater than or equal to the deviation threshold, adjust a contribution value corresponding to each group in the property calculation model until the property calculation model converges.

43. The optimization apparatus according to claim 42, wherein the model training unit is configured to establish the property calculation model as shown below:

$$f = a + \sum_i n_i \Delta f_i ;$$

where, f is the physical property of the single molecule, n_i is the number of groups of the i-th group, Δf_i is the contribution value of the i-th group to the physical property, and a is an associated constant.

44. The optimization apparatus according to claim 42, wherein the model training unit is, in particular, configured to determine a primary group, the number of groups of the primary group, a multi-stage group, and the number of groups of the multi-stage group in all groups of the single molecule, take all groups constituting the single molecule as the primary group, take various groups which coexist and contribute to a same physical property in common as the multi-stage group, and take the number of the various groups as a level of the multi-stage group.

45. The optimization apparatus according to claim 44, wherein the model training unit is configured to establish the property calculation model as shown below:

$$f = a + \sum_i \mathrm{m}_{1i} \Delta f_{1i} + \sum_j m_{2j} \Delta f_{2j} ..... + \sum_l m_{Nl} \Delta f_{Nl} ;$$

where, f is the physical property of the single molecule, m_{1i} is the number of groups of the i-th group in the primary group, Δf_{1i} is the contribution value of the i-th group in the primary group to the physical property, m_{2j} is the number of groups of the j-th group in a secondary group, Δf_{2j} is the contribution value of the j-th group in the secondary group to the physical property, m_{Nl} is the number of groups of the l-th group in an N-stage group, Δf_{Nl} is the contribution value of the l-th group in the N-stage group to the physical property, a is an associated constant, and N is a positive integer greater than or equal to 2.

46. The optimization apparatus according to claim 40, wherein the first processing unit is, in particular, configured to determine a primary group, the number of groups of the primary group, a multi-stage group, and the number of groups of the multi-stage group in

all groups of the single molecule, take all groups constituting the single molecule as the primary group, take various groups which coexist and contribute to a same physical property in common as the multi-stage group, and take the number of the various groups as a level of the multi-stage group.

47. The optimization apparatus according to claim 46, wherein the first processing unit is, in particular, configured to calculate the boiling point of the single molecule according to the following the property calculation model:

$$T=\frac{SOL\times GROUP_1+SOL\times GROUP_2+.....+SOL\times GROUP_N}{(SOL\times N\text{umh})^d+b}+c;$$

where, T is the boiling point of the single molecule, SOL is a single molecule vector converted according to the number of groups of each group constituting the single molecule, $GROUP_{11}$ is a first contribution value vector converted according to a contribution value of the primary group to the boiling point, $GROUP_{12}$ is a second contribution value vector converted according to a contribution value of the secondary group to the boiling point, $GROUP_{1N}$ is an N-th contribution value vector converted according to a contribution value of the N-stage group to the boiling point, $N\text{umh}$ is the number of atoms other than the hydrogen atom in the single molecule, d is a first preset constant, b is a second preset constant, c is a third preset constant, and N is a positive integer greater than or equal to 2.

48. The optimization apparatus according to claim 47, wherein the first processing unit is, in particular, configured to take the number of species of groups as a dimension of the single molecule vector, and take the number of groups of each group as an element value of the corresponding dimension in the single molecule vector;

the first processing unit is, in particular, configured to take the number of types of primary groups as a dimension of the first contribution value vector, and take the contribution value of each primary group to the boiling point as an element value of the corresponding dimension in the first contribution value vector;

the first processing unit is, in particular, configured to take the number of types of secondary groups as a dimension of the second contribution value vector, and take the contribution value of each secondary group to the boiling point as an element value of the corresponding dimension in the second contribution value vector; and

the first processing unit is, in particular, configured to take the number of types of N-stage groups as a dimension of the N-th contribution value vector and take the contribution value of each N-stage group to the boiling point as an element value of the corresponding dimension in the N-th contribution value vector.

49. The optimization apparatus according to claim 29, wherein the first processing unit is, in particular, configured to obtain different amounts of each fraction according to the preset feedstock ratio, and respectively input each fraction into the product prediction model of the respective petroleum processing device, and the petroleum processing device comprises a catalytic cracking unit, a delayed coking unit, a residue hydrotreating unit, a hydrocracking unit, a diesel hydro-upgrading unit, a diesel hydro-refining unit, a gasoline hydro-refining unit, a catalytic reforming unit and an alkylation unit.

50. The optimization apparatus according to claim 49, wherein the optimization apparatus further comprises:

a model training unit configured to establish a product prediction model, acquire sample feedstock information for a sample feedstock, train the set of reaction rules by using the sample feedstock information, fix the set of reaction rules that has been trained; and train the reaction rate algorithm by using the sample feedstock information, and fixthe reaction rate algorithm that has been trained, to obtain the product prediction model that has been trained; wherein the product prediction model comprises: a set of reaction rules comprising a plurality of reaction rules and a reaction rate algorithm.

51. The optimization apparatus according to claim 50, wherein the sample feedstock information of the sample feedstock comprises: molecular composition of the sample feedstock, molecular content of each molecule in the sample feedstock, molecular composition of an actual product corresponding to the sample feedstock, and actual content of each molecule in the actual product.

52. The optimization apparatus according to claim 51, wherein the model training unit is, in particular, configured to process the molecular composition of the sample feedstock according to a preset set of reaction rules, to obtain a reaction pathway corresponding to each molecule in the molecular composition of the sample feedstock, obtain first molecule composition of a device output product comprising the sample feedstock, an intermediate product, and a predicted product according to the reaction path corresponding to each molecule in the molecular composition of the sample feedstock, in the device output product, comprising: the sample feedstock, the intermediate product, and the predicted

product, calculate a first relative deviation according to the first molecular composition of the device output product and second molecular composition of the actual product, if the first relative deviation meets a preset condition, fix the set of reaction rules, and, if the first relative deviation does not meet the preset condition, adjust a reaction rule in the set of reaction rules, and recalculate the first relative deviation according to the adjusted set of reaction rules until the first relative deviation meets the preset condition.

53. The optimization apparatus according to claim 52, wherein the model training unit is, in particular, configured to acquire species of single molecules in the first molecule composition, to constitute a first set, acquire species of single molecules in the second molecule composition, to constitute a second set, determine whether the second set is a subset of the first set, if the second set is not a subset of the first set, obtain a pre-stored relative deviation value that does not meet the preset condition as the first relative deviation, and, if the second set is a subset of the first set, calculate the first relative deviation by a calculating formula as follows:

$$x_1 = \frac{\text{card}\left((M - M_1 - M_2) - M_3\right)}{\text{card}\ (M - M_1 - M_2)}\ ;$$

where, x_1 is the first relative deviation, M is the first set, M_1 is a set of species of single molecules in the molecular composition of the sample feedstock, M_2 is a set of species of single molecules in the molecular composition of the intermediate product, M_3 is the second set, and card represents the number of elements in the sets.

54. The optimization apparatus according to claim 51, wherein the model training unit is, in particular, configured to calculate a reaction rate of a reaction path corresponding to each molecule in the molecular composition of the sample feedstock, respectively, according to the reaction rate algorithm, obtain predicted content of each molecule in the predicted product corresponding to the sample feedstock according to molecular content of each molecule in the sample feedstock and the reaction rate of the reaction path corresponding to the molecule, calculate a second relative deviation according to the predicted content of each molecule in the predicted product and the actual content of each molecule in the actual product, if the second relative deviation meets a preset condition, fix the reaction rate algorithm, and, if the second relative deviation does not meet the preset condition, adjust a parameter

in the reaction rate algorithm, and recalculate the second relative deviation according to the adjusted reaction rate algorithm until the second relative deviation meets the preset condition.

55. The optimization apparatus according to claim 54, wherein the model training unit is, in particular, configured to calculate a reaction rate of each reaction path according to a reaction rate constant in the reaction rate algorithm;

wherein the reaction rate constant is determined according to a calculation formula as follows:

$$k = \frac{k_B E}{h} \exp(\frac{E\Delta S - \Delta E}{RE}) \varphi \times P^{\alpha} ;$$

where, k is the reaction rate constant, k_B is the Boltzmann constant, h is the Planck constant, R is an ideal gas constant, E is a temperature value of the environment at which the reaction path is located, $\exp$ is an exponential function with base of natural constant, ΔS is an entropy change before and after the reaction corresponding to the reaction rule corresponding to the reaction path, ΔE is a reaction energy barrier corresponding to the reaction rule corresponding to the reaction path, φ is a catalyst activity factor, P is a pressure value of the environment at which the reaction path is located, and α is a pressure influencing factor corresponding to the reaction rule corresponding to the reaction path.

56. The optimization apparatus according to any one of claims 49-55, wherein each petroleum processing device corresponds to a set of reaction rules.

57. An optimization system for a whole process of molecular-level oil refinery comprising a processor, a communication interface, a memory, and a communication bus, wherein the processor, the communication interface, and the memory are in communication with each other via the communication bus;

the memory is configured to store a computer program; and

the processor is configured to carry out the method according to any one of claims 1-28 when executing the program stored in the memory.

58. A computer-readable storage medium, wherein the computer-readable storage medium has stored therein one or more programs, the one or more programs being executable by one or more processors to implement the method according to any one of claims 1-28.