Claims

1. A method for obtaining a production and processing scheme of petroleum processing, wherein the method comprises:

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;

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

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; each set of preset rules in the preset rule set includes the type and amount of the predicted product used; and

respectively calculating 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;

acquiring a preset standard set for a preset target product;

determining whether the product property of each of the mixed products meets a preset product property of a target mixed product obtained by blending corresponding each target product in the preset standard set;

if the preset product property is met, obtaining a target parameter according to all of the mixed products and determining whether the target parameter meets a preset condition; the target parameter is a content of substances in the product that will cause harm to the environment, or a proportion of products, which meet a preset standard, in all mixed products to all of the mixed products;

if the target parameter meets the preset condition, determining that the predicted product meets a preset standard for a target product corresponding to the predicted product in the preset standard set, and outputting the preset feedstock ratio, the pre-trained product prediction model and the preset rule set as a production and processing scheme; and using the

production and processing scheme to conduct petroleum processing in the actual production process; and

if the target parameter does not meet the preset condition, adjusting the operation parameter in the pre-trained 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 the preset product property and the target parameters in all of the mixed products meet the preset condition;

the operation parameter in the pre-trained product prediction model comprises a temperature of an environment where a reaction path in the pre-trained product prediction model is located, a pressure of an environment where a reaction path in the pre-trained product prediction model is located and space velocity.

2. The method according to claim 1, wherein the 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 pre-trained 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 method according to claim 1, wherein the adjusting an operation parameter in the pre-trained product prediction model comprises:

adjusting a temperature of an environment where a reaction path corresponding to the predicted product in the pre-trained product prediction model is located; and

re-obtaining the predicted molecular composition of the predicted product and the predicted molecular content of each single molecule in each of the predicted products according to the adjusted temperature.

4. The method according to claim 1, wherein the adjusting an operation parameter in the pre-trained product prediction model comprises:

adjusting a pressure of an environment where a reaction path corresponding to the predicted product in the pre-trained product prediction model is located; and

re-obtaining the predicted molecular composition of the predicted product and the predicted molecular content of each single molecule in each of the predicted products according to the adjusted pressure.

5. The method according to claim 1, wherein the respectively calculating 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 set of the product blending feedstocks and first component content of each single molecule in each set 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 set of the product blending feedstocks and the first component content of each single molecule in each set 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.

6. The method according to claim 5, 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;

wherein the pre-trained property calculation model is used to calculate the physical property of the single molecule according to the number of groups of each group contained in a single molecule and a contribution value of each group to the physical property.

7. The method according to claim 6, 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 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.

8. The method according to claim 6, 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 output 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 of each group to the physical property in the property calculation model which is converged, and storing the 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 of each group to the physical property in the property calculation model until the property calculation model converges.

9. The method according to claim 8, wherein the property calculation model is established as shown below:

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

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

10. The method according to claim 8, 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.

11. The method according to claim 10, 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.

12. The method according to claim 7, 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.

13. The method according to claim 12, wherein,

the physical property of the single molecule comprises a boiling point of a single molecule;

the calculating the physical property of the single molecule comprises: calculating the boiling point of the single molecule according to a property calculation model as follows:

$$T=\frac{SOL\times GROUP_{11}+SOL\times GROUP_{12}+.....+SOL\times GROUP_{1N}}{(SOL\times N\text{umh})^{d}+b}+c;$$

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.

14. The method according to claim 12, wherein,

the physical property of the single molecule comprises a density of a single molecule;

the calculating the physical property of the single molecule comprises:

calculating the density of the single molecule according to a property calculation model as follows:

$$D=\frac{SOL\times GROUP_{21}}{(SOL\times GROUP_{22}+.....+SOL\times GROUP_{2N})\times e};$$

where, D is the density of the single molecule, SOL is a single molecule vector converted according to the number of groups of each group constituting the single molecule, $GROUP_{21}$ is an N+1-th contribution value vector converted according to a contribution value of the primary group to the density, $GROUP_{22}$ is an N+2-th contribution value vector converted according to a contribution value of the secondary group to the density, $GROUP_{2N}$

is a 2N-th contribution value vector converted according to a contribution value of the N-stage group to the density, e is the fourth preset constant; and N is a positive integer greater than or equal to 2.

15. The method according to claim 12, wherein,

the physical property of the single molecule comprises an octane number of a single molecule;

the calculating the physical property of the single molecule comprises:

calculating the octane number of the single molecule according to a property calculation model as follows:

$$X = SOL \times GROUP_{31} + SOL \times GROUP_{32} + ... + SOL \times GROUP_{3N} + h;$$

where, X is the octane number of the single molecule, SOL is a single molecule vector converted according to the number of groups of each group constituting the single molecule, $GROUP_{31}$ is a 2N+1-th contribution value vector converted according to a contribution value of the primary group to the octane number, $GROUP_{32}$ is a 2N+2-th contribution value vector converted according to a contribution value of the secondary group to the octane number, $GROUP_{3N}$ is a 3N-ty contribution value vector converted according to a contribution value of the N-stage group to the octane number; N is a positive integer greater than or equal to 2; and h is the fifth preset constant.

16. The method according to claim 1, wherein,

the product property of the mixed products comprises a density, a cloud point, a pour point, an aniline point, and an octane number.

17. The method according to claim 16, wherein, when a product property of the mixed product is the density, calculating the product property of each of the mixed products comprises:

calculating the density of each of the mixed products according to a calculation formula as follows:

$$density = \sum (D_i \times x_{i_volume});$$

where, $density$ is the density of the mixed product, D_i is the density of the i-th single molecule, and x_{i_volume} is second component content of the i-th single molecule.

18. The method according to claim 16, wherein, when a product property of the mixed product is the cloud point, calculating the product property of each of the mixed products comprises:

for each mixed product, calculating a cloud point contribution value of each single molecule according to the density and the boiling point of each single molecule in the mixed product; and

calculating the cloud point of the mixed product according to cloud point contribution values of all of the single molecules and content of each single molecule in the mixed product.

19. The method according to claim 16, wherein, when a product property of the mixed product is the pour point, calculating the product property of each of the mixed products comprises:

for each mixed product, calculating a pour point contribution value of each single molecule according to the density and molecular weight of each single molecule in the mixed product; and

calculating the pour point of the mixed product according to pour point contribution values of all of the single molecules and content of each single molecule in the mixed product.

20. The method according to claim 16, wherein, when a product property of the mixed product is the aniline point, calculating the product property of each of the mixed products comprises:

for each mixed product, calculating an aniline point contribution value of each single molecule according to the density and the boiling point of each single molecule in the mixed product; and

calculating the aniline point of the mixed product according to aniline point contribution values of all of the single molecules and content of each single molecule in the mixed product.

21. The method according to claim 16, wherein, when a product property of the mixed product is the octane number, calculating the product property of each of the mixed products comprises:

for each mixed product, acquiring the octane number of each single molecule and content of each single molecule in the mixed product; and

calculating the octane number of the mixed products according to a calculation formula as follows:

$$\begin{aligned}\mathrm{ON} = (&\sum_{i=\mathrm{HISQFG}} \upsilon_i\beta_i\mathrm{ON}_i + \mathrm{C_H}\sum_{i=\mathrm{H}} \upsilon_i\beta_i\mathrm{ON}_i + \mathrm{C_I}\sum_{i=\mathrm{I}} \upsilon_i\beta_i\mathrm{ON}_i + \mathrm{C_S}\sum_{i=\mathrm{S}} \upsilon_i\beta_i\mathrm{ON}_i \\ &+ \mathrm{C_Q}\sum_{i=\mathrm{Q}} \upsilon_i\beta_i\mathrm{ON}_i + \mathrm{C_F}\sum_{i=\mathrm{F}} \upsilon_i\beta_i\mathrm{ON}_i + \mathrm{C_G}\sum_{i=\mathrm{G}} \upsilon_i\beta_i\mathrm{ON}_i) \div \\ &(\sum_{i=\mathrm{HISQFG}} \upsilon_i\beta_i + \mathrm{C_H}(\sum_{i=\mathrm{H}} \upsilon_i\beta_i - \sum_{i=\mathrm{H}} \upsilon_i) + \mathrm{C_I}(\sum_{i=\mathrm{I}} \upsilon_i\beta_i - \sum_{i=\mathrm{I}} \upsilon_i) + \mathrm{C_S}(\sum_{i=\mathrm{S}} \upsilon_i\beta_i - \sum_{i=\mathrm{S}} \upsilon_i) \\ &+ \mathrm{C_Q}(\sum_{i=\mathrm{Q}} \upsilon_i\beta_i - \sum_{i=\mathrm{Q}} \upsilon_i) + \mathrm{C_F}(\sum_{i=\mathrm{F}} \upsilon_i\beta_i - \sum_{i=\mathrm{F}} \upsilon_i) + \mathrm{C_G}(\sum_{i=\mathrm{G}} \upsilon_i\beta_i - \sum_{i=\mathrm{G}} \upsilon_i))\end{aligned};$$

$$\mathrm{C_H} = \frac{k_{\mathrm{HI}}^{(a)}\upsilon_{\mathrm{I}} + k_{\mathrm{HS}}^{(a)}\upsilon_{\mathrm{S}} + k_{\mathrm{HQ}}^{(a)}\upsilon_{\mathrm{Q}} + k_{\mathrm{HF}}^{(a)}\upsilon_{\mathrm{F}} + k_{\mathrm{HG}}^{(a)}\upsilon_{\mathrm{G}}}{1 + k_{\mathrm{HI}}^{(\mathrm{b})}\upsilon_{\mathrm{I}} + k_{\mathrm{HS}}^{(\mathrm{b})}\upsilon_{\mathrm{S}} + k_{\mathrm{HQ}}^{(\mathrm{b})}\upsilon_{\mathrm{Q}} + k_{\mathrm{HF}}^{(\mathrm{b})}\upsilon_{\mathrm{F}} + k_{\mathrm{HG}}^{(\mathrm{b})}\upsilon_{\mathrm{G}}};$$

$$\mathrm{C_I} = \frac{k_{\mathrm{HI}}^{(a)}\upsilon_{\mathrm{H}} + k_{\mathrm{IS}}^{(a)}\upsilon_{\mathrm{S}} + k_{\mathrm{IQ}}^{(a)}\upsilon_{\mathrm{Q}} + k_{\mathrm{IF}}^{(a)}\upsilon_{\mathrm{F}} + k_{\mathrm{IG}}^{(a)}\upsilon_{\mathrm{G}}}{1 + k_{\mathrm{HI}}^{(\mathrm{b})}\upsilon_{\mathrm{H}} + k_{\mathrm{IS}}^{(\mathrm{b})}\upsilon_{\mathrm{S}} + k_{\mathrm{IQ}}^{(\mathrm{b})}\upsilon_{\mathrm{Q}} + k_{\mathrm{IF}}^{(\mathrm{b})}\upsilon_{\mathrm{F}} + k_{\mathrm{IG}}^{(\mathrm{b})}\upsilon_{\mathrm{G}}};$$

$$\mathrm{C_S} = \frac{k_{\mathrm{HS}}^{(a)}\upsilon_{\mathrm{H}} + k_{\mathrm{IS}}^{(a)}\upsilon_{\mathrm{I}} + k_{\mathrm{SQ}}^{(a)}\upsilon_{\mathrm{Q}} + k_{SF}^{(a)}\upsilon_{\mathrm{F}} + k_{\mathrm{SG}}^{(a)}\upsilon_{\mathrm{G}}}{1 + k_{\mathrm{HS}}^{(\mathrm{b})}\upsilon_{\mathrm{H}} + k_{\mathrm{IS}}^{(\mathrm{b})}\upsilon_{\mathrm{I}} + k_{\mathrm{SQ}}^{(\mathrm{b})}\upsilon_{\mathrm{Q}} + k_{\mathrm{SF}}^{(\mathrm{b})}\upsilon_{\mathrm{F}} + k_{\mathrm{SG}}^{(\mathrm{b})}\upsilon_{\mathrm{G}}};$$

$$\mathrm{C_Q} = \frac{k_{HQ}^{(a)}\upsilon_{\mathrm{H}} + k_{\mathrm{IQ}}^{(a)}\upsilon_{\mathrm{I}} + k_{\mathrm{SQ}}^{(a)}\upsilon_{S} + k_{\mathrm{QF}}^{(a)}\upsilon_{\mathrm{F}} + k_{\mathrm{QG}}^{(a)}\upsilon_{\mathrm{G}}}{1 + k_{\mathrm{HQ}}^{(\mathrm{b})}\upsilon_{\mathrm{H}} + k_{\mathrm{IQ}}^{(\mathrm{b})}\upsilon_{\mathrm{I}} + k_{\mathrm{SQ}}^{(\mathrm{b})}\upsilon_{\mathrm{S}} + k_{\mathrm{QF}}^{(\mathrm{b})}\upsilon_{\mathrm{F}} + k_{\mathrm{QG}}^{(\mathrm{b})}\upsilon_{\mathrm{G}}};$$

$$\mathrm{C_F} = \frac{k_{\mathrm{HF}}^{(a)}\upsilon_{\mathrm{H}} + k_{\mathrm{IF}}^{(a)}\upsilon_{\mathrm{I}} + k_{\mathrm{SF}}^{(a)}\upsilon_{\mathrm{S}} + k_{\mathrm{QF}}^{(a)}\upsilon_{Q} + k_{\mathrm{FG}}^{(a)}\upsilon_{\mathrm{G}}}{1 + k_{\mathrm{HF}}^{(\mathrm{b})}\upsilon_{\mathrm{H}} + k_{\mathrm{IF}}^{(\mathrm{b})}\upsilon_{\mathrm{I}} + k_{\mathrm{SF}}^{(\mathrm{b})}\upsilon_{\mathrm{S}} + k_{\mathrm{QF}}^{(\mathrm{b})}\upsilon_{\mathrm{Q}} + k_{\mathrm{FG}}^{(\mathrm{b})}\upsilon_{\mathrm{G}}};$$

$$\mathrm{C_G} = \frac{k_{\mathrm{HG}}^{(a)}\upsilon_{\mathrm{H}} + k_{\mathrm{IG}}^{(a)}\upsilon_{\mathrm{I}} + k_{\mathrm{SG}}^{(a)}\upsilon_{\mathrm{S}} + k_{\mathrm{QG}}^{(a)}\upsilon_{\mathrm{Q}} + k_{\mathrm{FG}}^{(a)}\upsilon_{\mathrm{F}}}{1 + k_{HG}^{(\mathrm{b})}\upsilon_{\mathrm{H}} + k_{\mathrm{IG}}^{(\mathrm{b})}\upsilon_{\mathrm{I}} + k_{\mathrm{SG}}^{(\mathrm{b})}\upsilon_{\mathrm{S}} + k_{\mathrm{QG}}^{(\mathrm{b})}\upsilon_{\mathrm{Q}} + k_{FG}^{(\mathrm{b})}\upsilon_{\mathrm{F}}};$$

where, ON is the octane number of the mixed product, HISQFG is a molecular collection, H is a molecular set of n-alkanes, I is a molecular set of isoalkanes, S is a molecular set of cycloalkanes, Q is a molecular set of olefins, F is a molecular set of aromatic hydrocarbons, G is a molecular set of oxygenated compounds, υ_i is content of each molecule in the mixed product, υ_{H}, υ_{I}, υ_{S}, υ_{Q}, υ_{F} and υ_{G} are total content of n-alkanes, total content of isoalkanes, total content of cycloalkanes, total content of olefins, total content of aromatic hydrocarbons, and total content of a compound of oxygenated compounds in the mixed product, respectively, β_i is a regression parameter of each molecule in the mixed product, ON_i is an octane number of each molecule in the mixed product, C_{H} is an interaction coefficient of n-alkanes with other molecules, C_{I} is an interaction coefficient of isoalkanes with other molecules; C_{S} is an interaction coefficient of cycloalkanes with other molecules; C_{Q} is an interaction coefficient of olefins with other molecules, C_{F} is an interaction

coefficient of aromatic hydrocarbons with other molecules, C_{G} is an interaction coefficient of oxygenated compounds with other molecules, $k_{\mathrm{HI}}^{(a)}$ is a first constant coefficient between n-alkanes and isoalkanes, $k_{\mathrm{HS}}^{(a)}$ is a first constant coefficient between n-alkanes and cycloalkanes, $k_{\mathrm{HQ}}^{(a)}$ is a first constant coefficient between n-alkanes and olefins, $k_{\mathrm{HF}}^{(a)}$ is a first constant coefficient between n-alkanes and aromatic hydrocarbons, $k_{HG}^{(a)}$ is a first constant coefficient between n-alkanes and oxygenated compounds, $k_{\mathrm{IS}}^{(a)}$ is a first constant coefficient between isoalkanes and cycloalkanes, $k_{\mathrm{IQ}}^{(a)}$ is a first constant coefficient between isoalkanes and olefins, $k_{\mathrm{IF}}^{(a)}$ is a first constant coefficient between isoalkanes and aromatic hydrocarbons, $k_{\mathrm{IG}}^{(a)}$ is a first constant coefficient between isoalkanes and oxygenated compounds, $k_{\mathrm{SQ}}^{(a)}$ is a first constant coefficient between cycloalkanes and olefins, $k_{\mathrm{SF}}^{(a)}$ is a first constant coefficient between cycloalkanes and aromatic hydrocarbons, $k_{\mathrm{SG}}^{(a)}$ is a first constant coefficient between cycloalkanes and oxygenated compounds, $k_{\mathrm{QF}}^{(a)}$ is a first constant coefficient between olefins and aromatic hydrocarbons, $k_{\mathrm{QG}}^{(a)}$ is a second constant coefficient between olefins and oxygenated compounds, $k_{\mathrm{FG}}^{(a)}$ is a first constant coefficient between aromatic hydrocarbons and oxygenated compounds, $k_{\mathrm{HI}}^{(\mathrm{b})}$ is a second constant coefficient between n-alkanes and isoalkanes, $k_{\mathrm{HS}}^{(\mathrm{b})}$ is a second constant coefficient between n-alkanes and cycloalkanes, $k_{\mathrm{HQ}}^{(\mathrm{b})}$ is a second constant coefficient between n-alkanes and olefins, $k_{\mathrm{HF}}^{(\mathrm{b})}$ is a second constant coefficient between n-alkanes and aromatic hydrocarbons, $k_{\mathrm{HG}}^{(\mathrm{b})}$ is a second constant coefficient between n-alkanes and oxygenated compounds, $k_{\mathrm{IS}}^{(\mathrm{b})}$ is a second constant coefficient between isoalkanes and cycloalkanes, $k_{\mathrm{IQ}}^{(\mathrm{b})}$ is a second constant coefficient between isoalkanes and olefins, $k_{\mathrm{IF}}^{(\mathrm{b})}$ is a second constant coefficient between isoalkanes and aromatic hydrocarbons, $k_{\mathrm{IG}}^{(\mathrm{b})}$ is a second constant coefficient between isoalkanes and oxygenated compounds, $k_{\mathrm{SQ}}^{(\mathrm{b})}$ is a second constant coefficient between cycloalkanes and olefins, $k_{\mathrm{SF}}^{(\mathrm{b})}$ is a second constant coefficient between cycloalkanes and aromatic

hydrocarbons, $k_{SG}^{(b)}$ ris a second constant coefficient between cycloalkanes and oxygenated compound, $k_{QF}^{(b)}$ is a second constant coefficient between olefins and aromatic hydrocarbons, $k_{QG}^{(b)}$ is a second constant coefficient between olefins and oxygenated compound, and $k_{FG}^{(b)}$ is a second constant coefficient between aromatic hydrocarbons and oxygenated compound; wherein the octane number comprises: a research octane number and a motor octane number.

22. The method according to claim 1, 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 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 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 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 is the number of elements in the sets.

26. The 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 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:

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

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 method according to claim 1, wherein types of the pre-trained product prediction model corresponding to a petroleum processing device comprise:

a pre-trained product prediction model corresponding to a catalytic cracking unit, a pre-trained product prediction model corresponding to a delayed coking unit, a pre-trained product prediction model corresponding to a residue hydrotreating unit, a pre-trained product prediction model corresponding to a hydrocracking unit, a pre-trained product prediction model corresponding to a diesel hydro-upgrading unit, a pre-trained product prediction model corresponding to a diesel hydro-refining unit, a pre-trained product prediction model

corresponding to a gasoline hydro-refining unit, a pre-trained product prediction model corresponding to a catalytic reforming unit and a pre-trained product prediction model corresponding to an alkylation unit.

29. An apparatus for obtaining a production and processing scheme of petroleum processing, wherein the apparatus comprises:

a first acquisition unit (11) configured to acquire molecular composition of crude oil;

a first processing unit (12) 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;

a second processing unit (13) configured to serve the corresponding fractions as petroleum processing feedstocks, and respectively input, according to a preset feedstock ratio, the molecular composition of the corresponding fractions into a pre-trained product prediction model corresponding to a petroleum processing device, to obtain predicted molecular composition of a corresponding predicted product output by the pre-trained product prediction model and predicted molecular content of each single molecule in the predicted molecular composition;

a product blending 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, and respectively calculate 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; each set of preset rules in the preset rule set includes the type and amount of the predicted product used;

a second acquisition unit (14) configured to acquire a preset standard set for a preset target product; and

a third processing unit (15) configured to determine whether the product property of each of the mixed products meets a preset product property of a target mixed product obtained by blending corresponding each target product in the preset standard set; if the preset product property is met, obtain a target parameter according to all of the mixed products and determining whether the target parameter meets a preset condition; if the target parameter meets the preset condition, determine that the predicted product meets a preset standard for a target product corresponding to the predicted product in the preset standard set, and output the preset feedstock ratio, the pre-trained product prediction model and the preset rule set as a production and processing scheme, and use the production and processing

scheme to conduct petroleum processing in the actual production process; and if the target parameter does not meet the preset condition, adjust the operation parameter in the pre-trained 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 the preset product property and the target parameters in all of the mixed products meet the preset condition; the target parameter is a content of substances in the product that will cause harm to the environment, or a proportion of products, which meet a preset standard, in all mixed products to all of the mixed products; the operation parameter in the pre-trained product prediction model comprises the operation parameter comprises a temperature of an environment where a reaction path in the pre-trained product prediction model is located, a pressure of an environment where a reaction path in the pre-trained product prediction model is located and space velocity.

30. The apparatus according to claim 29, wherein the 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, 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 pre-trained 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 apparatus according to claim 29, wherein the third processing unit (15), in particular, is configured to adjust a temperature of an environment where a reaction path corresponding to the predicted product in the pre-trained product prediction model is located, and re-obtain the predicted molecular composition of the predicted product and the predicted molecular content of each single molecule in each of the predicted products according to the adjusted temperature.

32. The apparatus according to claim 29, wherein the third processing unit (15), in particular, is configured to adjust a pressure of an environment where a reaction path corresponding to the predicted product in the pre-trained product prediction model is located, and re-obtain the predicted molecular composition of the predicted product and the predicted molecular content of each single molecule in each of the predicted products according to the adjusted pressure.

33. The apparatus according to claim 32, wherein the product blending unit, in particular, is configured to acquire first molecular composition of each set of the product blending feedstocks and first component content of each single molecule in each set 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 set of the product blending feedstocks and the first component content of each single molecule in each set 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.

34. The apparatus according to claim 33, wherein the product blending unit, in particular, is 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; wherein the pre-trained property calculation model is used to calculate the physical property of the single molecule according to the number of groups of each group contained in a single molecule and a contribution value of each group to the physical property.

35. The apparatus according to claim 34, wherein the 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, by the product blending unit, perform 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.

36. The apparatus according to claim 34, wherein the 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 output 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 of each group to the physical property in the property calculation model which is converged, and store the 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 of each group to the physical property in the property calculation model until the property calculation model converges.

37. The apparatus according to claim 36, wherein the model training unit, in particular, is configured to establish the property calculation model as shown below:

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

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

38. The apparatus according to claim 36, wherein the model training unit, in particular, is 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, and 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.

39. The apparatus according to claim 38, wherein the model training unit, in particular, 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.

40. The apparatus according to claim 35, wherein the product blending unit, in particular, is 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, and 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.

41. The apparatus according to claim 40, wherein the product blending unit, in particular, is configured to calculate a boiling point of the single molecule according to a property calculation model as follows:

$$T=\frac{SOL\times GROUP_{11}+SOL\times GROUP_{12}+.....+SOL\times GROUP_{1N}}{(SOL\times N\text{umh})^{d}+b}+c;$$

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.

42. The apparatus according to claim 40, wherein the product blending unit, in particular, is configured to calculate a density of the single molecule according to a property calculation model as follows:

$$D = \frac{SOL \times GROUP_{21}}{(SOL \times GROUP_{22} + ... + SOL \times GROUP_{2N}) \times e};$$

where, D is the density of the single molecule, SOL is a single molecule vector converted according to the number of groups of each group constituting the single molecule, $GROUP_{21}$ is an N+1-th contribution value vector converted according to a contribution value of the primary group to the density, $GROUP_{22}$ is an N+2-th contribution value vector converted according to a contribution value of the secondary group to the density, $GROUP_{2N}$ is a 2N-th contribution value vector converted according to a contribution value of the N-stage group to the density, e is the fourth preset constant; and N is a positive integer greater than or equal to 2.

43. The apparatus according to claim 40, wherein the product blending unit, in particular, is configured to calculate an octane number of the single molecule according to a property calculation model as follows:

$$X = SOL \times GROUP_{31} + SOL \times GROUP_{32} + ... + SOL \times GROUP_{3N} + h;$$

where, X is the octane number of the single molecule, SOL is a single molecule vector converted according to the number of groups of each group constituting the single molecule, $GROUP_{31}$ is a 2N+1-th contribution value vector converted according to a contribution value of the primary group to the octane number, $GROUP_{32}$ is a 2N+2-th contribution value vector converted according to a contribution value of the secondary group to the octane number, $GROUP_{3N}$ is a 3N-ty contribution value vector converted according to a contribution value of the N-stage group to the octane number; N is a positive integer greater than or equal to 2; and h is the fifth preset constant.

44. The apparatus according to claim 29, wherein the product property of the mixed products comprises a density, a cloud point, a pour point, an aniline point, and an octane number.

45. The apparatus according to claim 44, wherein the product blending unit, in particular, is configured to calculate the density of each of the mixed products according to a calculation formula as follows:

$$density = \sum (D_i \times x_{i_volume});$$

where, $density$ is the density of the mixed product, D_i is the density of the i-th single molecule, and x_{i_volume} is second component content of the i-th single molecule.

46. The apparatus according to claim 44, wherein the product blending unit, in particular, is configured to, for each mixed product, calculate a cloud point contribution value of each single molecule according to the density and the boiling point of each single molecule in the mixed product, and calculate the cloud point of the mixed product according to cloud point contribution values of all of the single molecules and content of each single molecule in the mixed product.

47. The apparatus according to claim 44, wherein the product blending unit, in particular, is configured to, for each mixed product, calculate a pour point contribution value of each single molecule according to the density and molecular weight of each single molecule in the mixed product, and calculate the pour point of the mixed product according to pour point contribution values of all of the single molecules and content of each single molecule in the mixed product.

48. The apparatus according to claim 44, wherein the product blending unit, in particular, is configured to, for each mixed product, calculate an aniline point contribution value of each single molecule according to the density and the boiling point of each single molecule in the mixed product, and calculate the aniline point of the mixed product according to aniline point contribution values of all of the single molecules and content of each single molecule in the mixed product.

49. The apparatus according to claim 44, wherein the product blending unit, in particular, is configured to, for each mixed product, acquire the octane number of each single molecule and content of each single molecule in the mixed product, and calculate the octane number of the mixed products according to a calculation formula as follows:

$$\begin{aligned}
\mathrm{ON} = (&\sum_{i=\mathrm{HISQFG}} \upsilon_i \beta_i \mathrm{ON}_i + \mathrm{C_H} \sum_{i=\mathrm{H}} \upsilon_i \beta_i \mathrm{ON}_i + \mathrm{C_I} \sum_{i=\mathrm{I}} \upsilon_i \beta_i \mathrm{ON}_i + \mathrm{C_S} \sum_{i=\mathrm{S}} \upsilon_i \beta_i \mathrm{ON}_i \\
&+ \mathrm{C_Q} \sum_{i=\mathrm{Q}} \upsilon_i \beta_i \mathrm{ON}_i + \mathrm{C_F} \sum_{i=\mathrm{F}} \upsilon_i \beta_i \mathrm{ON}_i + \mathrm{C_G} \sum_{i=\mathrm{G}} \upsilon_i \beta_i \mathrm{ON}_i) \div \\
(&\sum_{i=\mathrm{HISQFG}} \upsilon_i \beta_i + \mathrm{C_H}(\sum_{i=\mathrm{H}} \upsilon_i \beta_i - \sum_{i=\mathrm{H}} \upsilon_i) + \mathrm{C_I}(\sum_{i=\mathrm{I}} \upsilon_i \beta_i - \sum_{i=\mathrm{I}} \upsilon_i) + \mathrm{C_S}(\sum_{i=\mathrm{S}} \upsilon_i \beta_i - \sum_{i=\mathrm{S}} \upsilon_i) \\
&+ \mathrm{C_Q}(\sum_{i=\mathrm{Q}} \upsilon_i \beta_i - \sum_{i=\mathrm{Q}} \upsilon_i) + \mathrm{C_F}(\sum_{i=\mathrm{F}} \upsilon_i \beta_i - \sum_{i=\mathrm{F}} \upsilon_i) + \mathrm{C_G}(\sum_{i=\mathrm{G}} \upsilon_i \beta_i - \sum_{i=\mathrm{G}} \upsilon_i))
\end{aligned};$$

$$C_H = \frac{k_{HI}^{(a)}\upsilon_I + k_{HS}^{(a)}\upsilon_S + k_{HQ}^{(a)}\upsilon_Q + k_{HF}^{(a)}\upsilon_F + k_{HG}^{(a)}\upsilon_G}{1 + k_{HI}^{(b)}\upsilon_I + k_{HS}^{(b)}\upsilon_S + k_{HQ}^{(b)}\upsilon_Q + k_{HF}^{(b)}\upsilon_F + k_{HG}^{(b)}\upsilon_G};$$

$$C_I = \frac{k_{HI}^{(a)}\upsilon_H + k_{IS}^{(a)}\upsilon_S + k_{IQ}^{(a)}\upsilon_Q + k_{IF}^{(a)}\upsilon_F + k_{IG}^{(a)}\upsilon_G}{1 + k_{HI}^{(b)}\upsilon_H + k_{IS}^{(b)}\upsilon_S + k_{IQ}^{(b)}\upsilon_Q + k_{IF}^{(b)}\upsilon_F + k_{IG}^{(b)}\upsilon_G};$$

$$C_S = \frac{k_{HS}^{(a)}\upsilon_H + k_{IS}^{(a)}\upsilon_I + k_{SQ}^{(a)}\upsilon_Q + k_{SF}^{(a)}\upsilon_F + k_{SG}^{(a)}\upsilon_G}{1 + k_{HS}^{(b)}\upsilon_H + k_{IS}^{(b)}\upsilon_I + k_{SQ}^{(b)}\upsilon_Q + k_{SF}^{(b)}\upsilon_F + k_{SG}^{(b)}\upsilon_G};$$

$$C_Q = \frac{k_{HQ}^{(a)}\upsilon_H + k_{IQ}^{(a)}\upsilon_I + k_{SQ}^{(a)}\upsilon_S + k_{QF}^{(a)}\upsilon_F + k_{QG}^{(a)}\upsilon_G}{1 + k_{HQ}^{(b)}\upsilon_H + k_{IQ}^{(b)}\upsilon_I + k_{SQ}^{(b)}\upsilon_S + k_{QF}^{(b)}\upsilon_F + k_{QG}^{(b)}\upsilon_G};$$

$$C_F = \frac{k_{HF}^{(a)}\upsilon_H + k_{IF}^{(a)}\upsilon_I + k_{SF}^{(a)}\upsilon_S + k_{QF}^{(a)}\upsilon_Q + k_{FG}^{(a)}\upsilon_G}{1 + k_{HF}^{(b)}\upsilon_H + k_{IF}^{(b)}\upsilon_I + k_{SF}^{(b)}\upsilon_S + k_{QF}^{(b)}\upsilon_Q + k_{FG}^{(b)}\upsilon_G};$$

$$C_G = \frac{k_{HG}^{(a)}\upsilon_H + k_{IG}^{(a)}\upsilon_I + k_{SG}^{(a)}\upsilon_S + k_{QG}^{(a)}\upsilon_Q + k_{FG}^{(a)}\upsilon_F}{1 + k_{HG}^{(b)}\upsilon_H + k_{IG}^{(b)}\upsilon_I + k_{SG}^{(b)}\upsilon_S + k_{QG}^{(b)}\upsilon_Q + k_{FG}^{(b)}\upsilon_F};$$

where, ON is the octane number of the mixed product, HISQFG is a molecular collection, H is a molecular set of n-alkanes, I is a molecular set of isoalkanes, S is a molecular set of cycloalkanes, Q is a molecular set of olefins, F is a molecular set of aromatic hydrocarbons, G is a molecular set of oxygenated compounds, υ_i is content of each molecule in the mixed product, υ_H, υ_I, υ_S, υ_Q, υ_F and υ_G are total content of n-alkanes, total content of isoalkanes, total content of cycloalkanes, total content of olefins, total content of aromatic hydrocarbons, and total content of a compound of oxygenated compounds in the mixed product, respectively, β_i is a regression parameter of each molecule in the mixed product, ON_i is an octane number of each molecule in the mixed product, C_H is an interaction coefficient of n-alkanes with other molecules, C_I is an interaction coefficient of isoalkanes with other molecules; C_S is an interaction coefficient of cycloalkanes with other molecules; C_Q is an interaction coefficient of olefins with other molecules, C_F is an interaction coefficient of aromatic hydrocarbons with other molecules, C_G is an interaction coefficient of oxygenated compounds with other molecules, $k_{HI}^{(a)}$ is a first constant coefficient between n-alkanes and isoalkanes, $k_{HS}^{(a)}$ is a first constant coefficient between n-alkanes and cycloalkanes, $k_{HQ}^{(a)}$ is a first constant coefficient between n-alkanes and olefins, $k_{HF}^{(a)}$ is a first

constant coefficient between n-alkanes and aromatic hydrocarbons, $k_{HG}^{(a)}$ is a first constant coefficient between n-alkanes and oxygenated compounds, $k_{\mathrm{IS}}^{(a)}$ is a first constant coefficient between isoalkanes and cycloalkanes, $k_{\mathrm{IQ}}^{(a)}$ is a first constant coefficient between isoalkanes and olefins, $k_{\mathrm{IF}}^{(a)}$ is a first constant coefficient between isoalkanes and aromatic hydrocarbons, $k_{\mathrm{IG}}^{(a)}$ is a first constant coefficient between isoalkanes and oxygenated compounds, $k_{\mathrm{SQ}}^{(a)}$ is a first constant coefficient between cycloalkanes and olefins, $k_{\mathrm{SF}}^{(a)}$ is a first constant coefficient between cycloalkanes and aromatic hydrocarbons, $k_{\mathrm{SG}}^{(a)}$ is a first constant coefficient between cycloalkanes and oxygenated compounds, $k_{\mathrm{QF}}^{(a)}$ is a first constant coefficient between olefins and aromatic hydrocarbons, $k_{\mathrm{QG}}^{(a)}$ is a second constant coefficient between olefins and oxygenated compounds, $k_{\mathrm{FG}}^{(a)}$ is a first constant coefficient between aromatic hydrocarbons and oxygenated compounds, $k_{\mathrm{HI}}^{(\mathrm{b})}$ is a second constant coefficient between n-alkanes and isoalkanes, $k_{\mathrm{HS}}^{(\mathrm{b})}$ is a second constant coefficient between n-alkanes and cycloalkanes, $k_{\mathrm{HQ}}^{(\mathrm{b})}$ is a second constant coefficient between n-alkanes and olefins, $k_{\mathrm{HF}}^{(\mathrm{b})}$ is a second constant coefficient between n-alkanes and aromatic hydrocarbons, $k_{\mathrm{HG}}^{(\mathrm{b})}$ is a second constant coefficient between n-alkanes and oxygenated compounds, $k_{\mathrm{IS}}^{(\mathrm{b})}$ is a second constant coefficient between isoalkanes and cycloalkanes, $k_{\mathrm{IQ}}^{(\mathrm{b})}$ is a second constant coefficient between isoalkanes and olefins, $k_{\mathrm{IF}}^{(\mathrm{b})}$ is a second constant coefficient between isoalkanes and aromatic hydrocarbons, $k_{\mathrm{IG}}^{(\mathrm{b})}$ is a second constant coefficient between isoalkanes and oxygenated compounds, $k_{\mathrm{SQ}}^{(\mathrm{b})}$ is a second constant coefficient between cycloalkanes and olefins, $k_{\mathrm{SF}}^{(\mathrm{b})}$ is a second constant coefficient between cycloalkanes and aromatic hydrocarbons, $k_{\mathrm{SG}}^{(\mathrm{b})}$ is a second constant coefficient between cycloalkanes and oxygenated compound, $k_{\mathrm{QF}}^{(\mathrm{b})}$ is a second constant coefficient between olefins and aromatic hydrocarbons, $k_{\mathrm{QG}}^{(\mathrm{b})}$ is a second constant coefficient between olefins and oxygenated compound, and $k_{\mathrm{FG}}^{(\mathrm{b})}$ is a

second constant coefficient between aromatic hydrocarbons and oxygenated compound; wherein the octane number comprises: a research octane number and a motor octane number.

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

a model training unit configure to establish 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, acquire sample feedstock information for a sample feedstock, train the set of reaction rules by using the sample feedstock information, and fix the set of reaction rules that has been trained, and train the reaction rate algorithm by using the sample feedstock information, and fix the reaction rate algorithm that has been trained, to obtain the product prediction model that has been trained.

51. The 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 apparatus according to claim 51, wherein the model training unit, in particular, is 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 apparatus according to claim 52, wherein the model training unit, in particular, is 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 is the number of elements in the sets.

54. The apparatus according to claim 51, wherein the model training unit, in particular, is 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 apparatus according to claim 54, wherein the model training unit, in particular, is 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:

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

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 apparatus according to claim 29, wherein types of the pre-trained product prediction model corresponding to a petroleum processing device comprise: a pre-trained product prediction model corresponding to a catalytic cracking unit, a pre-trained product prediction model corresponding to a delayed coking unit, a pre-trained product prediction model corresponding to a residue hydrotreating unit, a pre-trained product prediction model corresponding to a hydrocracking unit, a pre-trained product prediction model corresponding to a diesel hydro-upgrading unit, a pre-trained product prediction model corresponding to a diesel hydro-refining unit, a pre-trained product prediction model corresponding to a gasoline hydro-refining unit, a pre-trained product prediction model corresponding to a catalytic reforming unit and an alkylation unit.

57. A system for obtaining a production and processing scheme of petroleum processing, wherein the system for obtaining a production and processing scheme of petroleum processing comprises a processor (210) and a memory (211), wherein the processor (210) is configured to execute a program of obtaining a production and processing scheme of petroleum processing stored in the memory (211) to implement a method for obtaining a production and processing scheme of petroleum processing of claim 1.

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 executed by one or more processors (210) to implement a method for obtaining a production and processing scheme of petroleum processing of claim 1.