

CIRCULATING STREAM UNBLOCKING METHOD FOR PROCESS SIMULATION

TECHNICAL FIELD

The present invention relates to the technical field of chemical process simulation, and in particular, to a method for closing a recycle stream in a process simulation.

BACKGROUND TECHNOLOGY

The conventional method for closing a recycle stream in a steady-state process simulation software includes the following steps: first, tearing a recycle stream into a recycle-inlet stream and a recycle-outlet stream; then, assigning an initial value to the recycle-inlet stream and performing solving; comparing information of the two streams after the solving; if results of the two streams are consistent, merging the two streams into one stream, thereby closing the recycle stream.

However, if the results of the two streams are significantly different, the result of the recycle-outlet stream is used as the initial value for the next operation to solve the recycle-inlet stream, and solving is performed repeatedly until the results of the two streams are relatively close to each other, thereby closing the recycle stream. The conventional method for closing the recycle stream in the steady-state process simulation software relies excessively on human experience in the determination of a tearing position for the recycle stream and the criterion for determining whether the information of the two streams is close. For systems with many components or relatively complex processes, as well as unreasonable position selections and unreasonable initial values, even a small deviation may cause a failure in closing the recycle stream, and it is difficult to handle the related problems by relying on human experience. In addition, for processes involving multiple recycles, when the conventional method is used to close a next recycle stream, a previously closed recycle stream may again fail to converge due to a change in conditions.

CONTENT OF THE INVENTION

In view of the above-mentioned shortcomings and deficiencies in the prior art, the present invention provides a method for closing a recycle stream in a process simulation.

To achieve the above objective, the main technical solutions adopted by the present invention are as follows:

An embodiment of the present invention provides a method for closing a recycle stream in a process simulation, including:

S1: obtaining an initial value of a feed stream and an initial value of a recycle stream in a rigorous mechanistic model corresponding to a specified chemical production process;

S2: obtaining, based on the initial value of the feed stream and the initial value of the recycle stream, deviation values of all streams in the rigorous mechanistic model;

S3: receiving a relaxation factor set by a user for any stream in the rigorous mechanistic model, taking the deviation value of the stream as a previous-round deviation value, and obtaining, based on the relaxation factor and the previous-round deviation value corresponding to the stream, a current-round deviation value and a current-round connection equation corresponding to the stream;

S4: combining the current-round connection equation corresponding to the stream with a pre-obtained first equation set to form a system of simultaneous equations, solving the system of simultaneous equations to obtain a solution result, and determining whether the solution result satisfies a convergence condition;

if the convergence condition is satisfied, then receiving a new relaxation factor obtained after the user adds an increment to the relaxation factor of the stream, taking the current-round deviation value corresponding to the stream as a new previous-round deviation value, and obtaining, based on the new relaxation factor and the new previous-round deviation value, a new current-round deviation value and a new current-round connection equation corresponding to the stream;

if the convergence condition is not satisfied, then receiving a new relaxation factor set by the user for the stream, and obtaining, based on the new relaxation factor and the previous-round deviation value, a new current-round deviation value and a new current-round connection equation corresponding to the stream; and

S5: repeating steps S4-S5 until the new current-round deviation value corresponding to the stream is 0.

Preferably, the S2 specifically includes:

S21: performing, based on the initial value of the feed stream and the initial value of the recycle stream, calculation on a module satisfying a first condition in the rigorous mechanistic model corresponding to the specified chemical production process to obtain an outlet variable of each module satisfying the first condition;

S22: obtaining, based on the outlet variable of any module satisfying the first condition, an inlet variable of a downstream module of the module;

S23: determining a module satisfying the first condition from among downstream modules of all modules satisfying the first condition, and obtaining, based on an inlet variable of the determined module, an outlet variable of the module; and

S24: repeating S22-S24 until an inlet variable and an outlet variable of each module and a deviation value of each stream in the rigorous mechanistic model corresponding to the specified chemical production process are obtained.

Preferably,

the first condition is that an inlet variable of the module is complete.

Preferably,

in the S24, the deviation value of the stream is equal to a difference obtained by subtracting an inlet variable of a downstream module of the stream from an outlet variable of an upstream module of the stream.

Preferably, the current-round deviation value corresponding to the stream in the S3 is obtained based on the relaxation factor and the previous-round deviation value corresponding to the stream by using Formula (1);

where Formula (1) is:

current-round deviation value = previous-round deviation value $\times$ (1 - relaxation

factor);

where the current-round connection equation corresponding to the stream is:

5 $0 = \text{outlet variable of the upstream module of the stream} - \text{inlet variable of the downstream module of the stream} - \text{current-round deviation value}.$

Preferably,

10 the first equation set includes current-round connection equations for all other streams, than the stream, in the rigorous mechanistic model corresponding to the specified chemical production process, and specified conditions corresponding to all modules in the specified chemical production process.

15 Preferably,

the convergence condition is that a residual of the system of simultaneous equations is less than a preset tolerance value.

20 Preferably, the method further includes:

S6: obtaining a connection equation corresponding to each stream in the rigorous mechanistic model corresponding to the current specified chemical production process, and then combining and solving the connection equation and the first equation set to obtain an
25 inlet flow rate of a downstream module of the recycle stream;

where the connection equation corresponding to each stream in the rigorous mechanistic model corresponding to the current specified chemical production process is: $0 = \text{outlet variable of the upstream module of the stream} - \text{inlet variable of the downstream module of the stream}.$
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Preferably,

in the S3, when the downstream module of the stream is a first module, the relaxation
35 factor set by the user for the stream is 0.5;

where the first module is any one of a heater, a flash tank, a mixer, and a splitter.

Preferably,

in the S4, when the solution result does not satisfy the convergence condition and the downstream module of the stream is the first module, the new relaxation factor set by the user for a first stream is received as 1; and when the downstream module of the stream is not the first module, the new relaxation factor obtained after the user adds a decrement to the relaxation factor of the stream is received.

The advantages of the present invention are as follows: the method for closing the recycle stream in the process simulation according to the present invention can obtain, based on the initial value of the feed stream and the initial value of the recycle stream, deviation values of all streams in the rigorous mechanistic model, receive a relaxation factor set by a user for any stream in the rigorous mechanistic model, take the deviation value of the stream as a previous-round deviation value, and obtain, based on the relaxation factor and the previous-round deviation value corresponding to the stream, a current-round deviation value and a current-round connection equation corresponding to the stream. Finally, the relaxation factors are continuously and simultaneously adjusted to gradually reduce the current-round deviation value to close the stream. The method can effectively reduce the repetitive work of a modeling personnel in closing a recycle stream, and improve the efficiency of closing the stream.

DESCRIPTION OF THE DRAWINGS

FIG. 1 is a flowchart of a method for closing a recycle stream in a process simulation according to the present invention.

FIG. 2 is a process flow diagram of a rigorous mechanistic model corresponding to a specified chemical production process in an embodiment of the present invention.

SPECIFIC IMPLEMENTATIONS

In order to better explain the present invention and facilitate the understanding of the present invention, the present invention is described in detail below with reference to the drawings and specific embodiments.

In order to better understand the above technical solution, exemplary embodiments of the present invention will be described in more detail below with reference to the drawings. Although the drawings show exemplary embodiments of the present invention, it should be understood that the present invention may be implemented in various forms and should not be limited to the embodiments set forth herein. On the contrary, these embodiments are provided so that the present invention can be more clearly and thoroughly understood, and the scope of the present invention can be fully conveyed to those skilled in the art.

It should be noted that the recycle stream refers to a stream that flows from an outlet back to an inlet and participates in a next treatment in a specified chemical production process.

Referring to FIG. 1, the present embodiment provides a method for closing a recycle stream in a process simulation, including:

S1: an initial value of a feed stream and an initial value of a recycle stream in a rigorous mechanistic model corresponding to a specified chemical production process are obtained.

In the present embodiment, both the initial value of the feed stream and the initial value of the recycle stream are set by a user.

In a specific application of the present embodiment, for example, referring to FIG. 2, which shows a process flow diagram of a rigorous mechanistic model corresponding to a specified chemical production process, B1, B2, B3, B4, and B5 are all modules in the rigorous mechanistic model, where each module represents a certain treatment process in the specified chemical production process. For example, a reactor module is configured to perform a chemical reaction, e.g., a batch reactor, a continuous flow reactor or the like; a distillation column module is configured to separate a mixture into different components through distillation; a separator vessel module is configured to separate a multiphase mixture into different phases, e.g., liquid-liquid separation or solid-liquid separation; and a compressor module is configured to compress a gas to increase a pressure, etc.. Specifically, each module has corresponding specified conditions. For example, the specified conditions (the specified conditions are manually preset and are used as calculation conditions for calculating a module execution process) for the reactor module include a specified reaction temperature, a pressure, a reactor volume, and a corresponding reaction thereof, as well as a calculation manner for the reactor module to execute the

corresponding process.

In FIG. 2, 2 represents a stream 2, 3 represents a stream 3, 6 represents a stream 6, 8 represents a stream 8, and so on. The module B1, the stream 2, the module B2, the stream 3, the module B3, and the stream 8 together form a recycle loop. The stream 8 is a recycle stream. 1 represents a feed stream 1, 5 represents a feed stream 5, 4 represents a discharge stream 4, and 7 represents a discharge stream 7. A stream is used to describe a connection relationship between various modules in a chemical process flow.

S2: based on the initial value of the feed stream and the initial value of the recycle stream, deviation values of all streams in the rigorous mechanistic model are obtained.

In a specific application of the present embodiment, the S2 specifically includes:

S21: based on the initial value of the feed stream and the initial value of the recycle stream, calculation is performed on a module satisfying a first condition in the rigorous mechanistic model corresponding to the specified chemical production process to obtain an outlet variable of each module satisfying the first condition.

The first condition is that an inlet variable of the module is complete. For example, the inlet variable of the module is complete, as shown in FIG. 2. The module B1 has two inlet variables, one being the feed stream 1 entering the module B1 and the other being the recycle stream 8 also entering the module B1. Since a user has set initial values for the two inlet variables, the inlet variables of the module B1 are complete at this time, and the module B1 satisfies the first condition. Similarly, the module B4 also satisfies the first condition at this time.

S22: based on the outlet variable of any module satisfying the first condition, an inlet variable of a downstream module of the module is obtained.

S23: a module satisfying the first condition is determined from among downstream modules of all modules satisfying the first condition, and an outlet variable of the module is obtained based on an inlet variable of the determined module.

S24: S22-S24 are repeated until an inlet variable and an outlet variable of each module and a deviation value of each stream in the rigorous mechanistic model corresponding to the specified

chemical production process are obtained.

In the S24, the deviation value of the stream is equal to a difference obtained by subtracting an inlet variable of a downstream module of the stream from an outlet variable of an upstream module of the stream.

In the present embodiment, for the rigorous mechanistic model corresponding to the specified chemical production process, complete calculation conditions are given by the user, where the calculation conditions include the specified conditions for each module and values of stream variables of the feed streams 1 and 5 and the recycle stream 8. Calculation is performed on modules satisfying the first condition (because the feed streams 1 and 5 have initial values and the recycle stream 8 also has an initial value, inlet variables of the module B1 are complete, that is, all inlet variables are known; similarly, an inlet variable of the module B4 is complete; thus, the module B1 and the module B4 satisfy the first condition) in the rigorous mechanistic model corresponding to the specified chemical production process to obtain an outlet variable of the module B1 and an outlet variable of the module B4, i.e., an upstream variable of the stream 2 and an upstream variable of the stream 6, and the outlet variable of the module B1 and the outlet variable of the module B4 are respectively used as an inlet variable of the module B2 and an inlet variable of the module B5. At this time, the inlet variable of the module B2 is complete, so that an upstream variable of the stream 3 and an upstream variable of the stream 9, i.e., outlet variables of the module B2, can be solved. Then, the upstream variable of the stream 3 and the upstream variable of the stream 9 are assigned to downstream variables. At this time, an inlet variable of the module B3 and inlet variables of the module B5 are complete, so that outlet variables of the module B3 and an outlet variable of the module B5 (i.e., an upstream variable of the stream 4, an upstream variable of the stream 7, and an upstream variable of the stream 8) can be solved.

S3: a relaxation factor set by a user for any stream in the rigorous mechanistic model is received, the deviation value of the stream is taken as a previous-round deviation value, and a current-round deviation value and a current-round connection equation corresponding to the stream are obtained based on the relaxation factor and the previous-round deviation value corresponding to the stream.

In a practical application of the present embodiment, the current-round deviation value corresponding to the stream in the S3 is obtained based on the relaxation factor and the

previous-round deviation value corresponding to the stream by using Formula (1).

Specifically, Formula (1) is:

5 $\text{current-round deviation value} = \text{previous-round deviation value} \times (1 - \text{relaxation factor}).$

Specifically, the current-round connection equation corresponding to the stream is:

10 $0 = \text{outlet variable of the upstream module of the stream} - \text{inlet variable of the downstream module of the stream} - \text{current-round deviation value}.$

For example, the deviation value of the stream 8 obtained in the S2 is taken as the previous-round deviation value. If the relaxation factor set by the user for the stream 8 is 0.2, then the current-round deviation value = previous-round deviation value $\times (1 - 0.2)$.

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S4: the current-round connection equation corresponding to the stream is combined with a pre-obtained first equation set to form a system of simultaneous equations, the system of simultaneous equations is solved to obtain a solution result, and it is determined whether the solution result satisfies a convergence condition.

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In the present embodiment, the first equation set includes current-round connection equations for all other streams, than the stream, in the rigorous mechanistic model corresponding to the specified chemical production process, and specified conditions corresponding to all modules in the specified chemical production process.

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The convergence condition is that a residual of the system of simultaneous equations is less than a preset tolerance value.

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If the convergence condition is satisfied, then a new relaxation factor obtained after the user adds an increment to the relaxation factor of the stream is received (i.e., the new relaxation factor obtained after the user adds the increment to the relaxation factor of the stream is received, for example, if the relaxation factor of the stream is 0.5, and the new relaxation factor obtained after the user adds the increment (such as 0.1) to the relaxation factor 0.5 of the stream is received, then the new relaxation factor is 0.6), the current-round deviation value corresponding to the stream is taken as a new previous-round deviation value, and a new current-round deviation

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value and a new current-round connection equation corresponding to the stream are obtained based on the new relaxation factor and the new previous-round deviation value.

If the convergence condition is not satisfied, then a new relaxation factor set by the user for the stream is received (i.e., one new relaxation factor set by the user for the stream is received), and a new current-round deviation value and a new current-round connection equation corresponding to the stream are obtained based on the new relaxation factor and the previous-round deviation value.

S5: steps S4-S5 are repeated until the new current-round deviation value corresponding to the stream is 0. In the present embodiment, when the new current-round deviation value is 0, the stream is considered closed.

In a practical application, the method further includes:

S6: a connection equation corresponding to each stream in the rigorous mechanistic model corresponding to the current specified chemical production process is obtained, and then the connection equation and the first equation set are combined and solved to obtain an inlet flow rate of a downstream module of the recycle stream.

Specifically, the connection equation corresponding to each stream in the rigorous mechanistic model corresponding to the current specified chemical production process is: $0 = \text{outlet variable of the upstream module of the stream} - \text{inlet variable of the downstream module of the stream}$.

In the present embodiment, after the stream is closed, the converged result obtained by solving the system of simultaneous equations when the previous new relaxation factor is 1 is loaded into the recycle stream 8 for which an initial value is given, so as to provide an initial value for the next solving and enable faster convergence.

In a specific implementation of the present embodiment, in the S3, when the downstream module of the stream is a first module, the relaxation factor set by the user for the stream is 0.5. Specifically, the first module is any one of a heater, a flash tank, a mixer, and a splitter.

In another specific implementation of the present embodiment, in the S4, when the solution

result does not satisfy the convergence condition and the downstream module of the stream is the first module, the new relaxation factor set by the user for a first stream is received as 1; and when the downstream module of the stream is not the first module, the new relaxation factor obtained after the user adds a decrement to the relaxation factor of the stream is received.

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In the present embodiment, when a user assigns values to relaxation factors of streams, the user may assign the same value to relaxation factors of all the streams uniformly, or for some relatively simple modules, the relaxation factors thereof may be quickly adjusted to 1 without causing the model to be non-convergence. For the inlet stream of the first module, the user automatically assigns a relaxation factor of 0.5 for the first time, and automatically assigns a relaxation factor of 1 for the second time in solving the system of simultaneous equations. This allows some streams to be closed quickly, thereby improving the overall model convergence. The relaxation factors for other modules are still configured uniformly by the user.

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The method for closing the recycle stream in the process simulation according to the present invention can obtain, based on the initial value of the feed stream and the initial value of the recycle stream, deviation values of all streams in the rigorous mechanistic model, receive a relaxation factor set by a user for any stream in the rigorous mechanistic model, take the deviation value of the stream as a previous-round deviation value, and obtain, based on the relaxation factor and the previous-round deviation value corresponding to the stream, a current-round deviation value and a current-round connection equation corresponding to the stream. Finally, the relaxation factors are continuously and simultaneously adjusted to gradually reduce the current-round deviation value to close the stream. The method can effectively reduce the repetitive work of a modeling personnel in closing a recycle stream, and improve the efficiency of closing the stream.

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In the description of the present invention, it should be understood that the terms “first” and “second” are used for descriptive purposes only and are not to be understood as indicating or implying relative importance or implicitly specifying the number of technical features indicated. Thus, a feature defined with “first” or “second” may expressly or implicitly include one or more of such features. In the description of the present invention, “plurality” means two or more, unless otherwise specifically defined.

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In the present invention, unless otherwise clearly specified and defined, terms such as “mount”, “connect”, “couple”, and “fix” should be interpreted in a broad sense. For example, the

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connection may be a fixed connection, a detachable connection, or an integral connection; it may be a mechanical connection or an electrical connection; it may be a direct connection or an indirect connection through an intermediate medium; or it may be a communication between the interiors of two components or an interaction between two components. For those having ordinary skill in the art, the specific meanings of the above terms in the present invention can be understood according to the specific circumstances.

In the present invention, unless otherwise clearly specified and defined, a first feature being “on” or “under” a second feature may mean that the first and second features are in direct contact, or that the first and second features are in indirect contact through an intermediate medium. Moreover, a first feature being “above”, “over”, or “on top of” a second feature may mean that the first feature is directly above or obliquely above the second feature, or simply means that the first feature has a higher horizontal level than the second feature. A first feature being “below”, “under”, or “beneath” a second feature may mean that the first feature is directly below or obliquely below the second feature, or simply means that the first feature has a lower horizontal level than the second feature.

In the description of the present specification, descriptions with reference to the terms “one embodiment”, “some embodiments”, “an embodiment”, “an example”, “a specific example”, or “some examples” mean that a specific feature, structure, material, or characteristic described in conjunction with the embodiment or example is included in at least one embodiment or example of the present invention. In the present specification, the schematic representations of the above terms do not necessarily refer to the same embodiment or example. Moreover, the specific features, structures, materials, or characteristics described may be combined in any suitable manner in any one or more of the embodiments or examples. Furthermore, those skilled in the art may combine and integrate different embodiments or examples described in the present specification, as well as features of different embodiments or examples on the premise of no mutual contradiction.

Although the embodiments of the present invention have been shown and described above, it should be understood that the above embodiments are exemplary and should not be construed as limiting the present invention. Those having ordinary skill in the art may make changes, modifications, substitutions, and variations to the above embodiments within the scope of the present invention.

CLAIMS

1. A method for closing a recycle stream in a process simulation, comprising:

5 S1: obtaining an initial value of a feed stream and an initial value of a recycle stream in a rigorous mechanistic model corresponding to a specified chemical production process;

S2: obtaining, based on the initial value of the feed stream and the initial value of the recycle stream, deviation values of all streams in the rigorous mechanistic model;

10 S3: receiving a relaxation factor set by a user for any stream in the rigorous mechanistic model, taking the deviation value of the stream as a previous-round deviation value, and obtaining, based on the relaxation factor and the previous-round deviation value corresponding to the stream, a current-round deviation value and a current-round connection equation
15 corresponding to the stream;

S4: combining the current-round connection equation corresponding to the stream with a pre-obtained first equation set to form a system of simultaneous equations, solving the system of simultaneous equations to obtain a solution result, and determining whether the solution result
20 satisfies a convergence condition;

if the convergence condition is satisfied, then receiving a new relaxation factor obtained after the user adds an increment to the relaxation factor of the stream, taking the current-round deviation value corresponding to the stream as a new previous-round
25 deviation value, and obtaining, based on the new relaxation factor and the new previous-round deviation value, a new current-round deviation value and a new current-round connection equation corresponding to the stream;

if the convergence condition is not satisfied, then receiving a new relaxation factor set
30 by the user for the stream, and obtaining, based on the new relaxation factor and the previous-round deviation value, a new current-round deviation value and a new current-round connection equation corresponding to the stream; and

S5: repeating steps S4-S5 until the new current-round deviation value corresponding to
35 the stream is 0.

2. The method for closing the recycle stream in the process simulation according to claim 1, wherein the S2 specifically comprises:

S21: performing, based on the initial value of the feed stream and the initial value of the recycle stream, calculation on a module satisfying a first condition in the rigorous mechanistic model corresponding to the specified chemical production process to obtain an outlet variable of each module satisfying the first condition;

S22: obtaining, based on the outlet variable of any module satisfying the first condition, an inlet variable of a downstream module of the module;

S23: determining a module satisfying the first condition from among downstream modules of all modules satisfying the first condition, and obtaining, based on an inlet variable of the determined module, an outlet variable of the module; and

S24: repeating S22-S24 until an inlet variable and an outlet variable of each module and a deviation value of each stream in the rigorous mechanistic model corresponding to the specified chemical production process are obtained.

3. The method for closing the recycle stream in the process simulation according to claim 2, wherein

the first condition is that an inlet variable of the module is complete.

4. The method for closing the recycle stream in the process simulation according to claim 3, wherein

in the S24, the deviation value of the stream is equal to a difference obtained by subtracting an inlet variable of a downstream module of the stream from an outlet variable of an upstream module of the stream.

5. The method for closing the recycle stream in the process simulation according to claim 4, wherein the current-round deviation value corresponding to the stream in the S3 is obtained based on the relaxation factor and the previous-round deviation value corresponding to the

stream by using Formula (1);

wherein Formula (1) is:

5 current-round deviation value = previous-round deviation value $\times$ (1 - relaxation factor);

wherein the current-round connection equation corresponding to the stream is:

10 0 = outlet variable of the upstream module of the stream - inlet variable of the downstream module of the stream - current-round deviation value.

6. The method for closing the recycle stream in the process simulation according to claim 5, wherein

15 the first equation set comprises current-round connection equations for all other streams, than the stream, in the rigorous mechanistic model corresponding to the specified chemical production process, and specified conditions corresponding to all modules in the specified chemical production process.

20 7. The method for closing the recycle stream in the process simulation according to claim 6, wherein

25 the convergence condition is that a residual of the system of simultaneous equations is less than a preset tolerance value.

8. The method for closing the recycle stream in the process simulation according to claim 7, wherein the method further comprises:

30 S6: obtaining a connection equation corresponding to each stream in the rigorous mechanistic model corresponding to the current specified chemical production process, and then combining and solving the connection equation and the first equation set to obtain an inlet flow rate of a downstream module of the recycle stream;

35 wherein the connection equation corresponding to each stream in the rigorous

mechanistic model corresponding to the current specified chemical production process is: $0 = \text{outlet variable of the upstream module of the stream} - \text{inlet variable of the downstream module of the stream}$.

- 5 9. The method for closing the recycle stream in the process simulation according to claim 8, wherein

in the S3, when the downstream module of the stream is a first module, the relaxation factor set by the user for the stream is 0.5;

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wherein the first module is any one of a heater, a flash tank, a mixer, and a splitter.

10. The method for closing the recycle stream in the process simulation according to claim 9, wherein

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in the S4, when the solution result does not satisfy the convergence condition and the downstream module of the stream is the first module, the new relaxation factor set by the user for a first stream is received as 1; and when the downstream module of the stream is not the first module, the new relaxation factor obtained after the user adds a decrement to the relaxation factor of the stream is received.

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