[0006] According to a first aspect of the present invention, there is provided a method, comprising: generating, by one or more processors, a plurality of training computational fluid dynamic (CFD) models for a plurality of training steady state mixing configurations in which inlet streams are mixed in tanks, wherein each training CFD model is generated based on a plurality of steady state mixing factors associated with each training steady state mixing configuration; calculating, by the one or more processors, a mixing quality for each training steady state mixing configuration using each respective training CFD model; generating, by the one or more processors, a training dataset that includes the steady state mixing factors associated with each training steady state mixing configuration, and the calculated mixing quality for each training steady state mixing configuration; training, by the one or more processors, a machine learning model, using the training dataset, to predict mixing qualities for steady state mixing configurations based on steady state mixing factors associated with the steady state mixing configurations; and recommending, by the one or more processors, one or more of a working volume or an impeller speed for a given product based on the trained machine learning model.

[0007] According to a second aspect of the present invention, there is provided a computer system, comprising: one or more processors; and a non-transitory program memory communicatively coupled to the one or more processors and storing executable instructions that, when executed by the one or more processors, cause the processors to: generate a plurality of training computational fluid dynamic (CFD) models for a plurality of training steady state mixing configurations in which inlet streams are mixed in tanks, wherein each training CFD model is generated based on a plurality of steady state mixing factors associated with each training steady state mixing configuration; calculate a mixing quality for each training steady state mixing configuration using each respective training CFD model; generate a training dataset that includes the steady state mixing factors associated with each training steady state mixing configuration, and the calculated mixing quality for each training steady state mixing configuration; train a machine learning model, using the training dataset, to predict mixing qualities for steady state mixing configurations based on steady state mixing factors associated with the steady state mixing configurations; and recommend one or more of a working volume or an impeller speed for a given product based on the trained machine learning model.

[0008] According to a third aspect of the present invention, there is provided a non-transitory computer readable storage medium storing computer-readable instructions that, when executed by one or more processors, cause the one or more processors to: generate a plurality of training computational fluid dynamic (CFD) models for a plurality of training steady state mixing configurations in which inlet streams are mixed in tanks, wherein each training CFD model is generated based on a plurality of steady state mixing factors associated with each training steady state mixing configuration; calculate a mixing quality for each training steady state mixing configuration using each respective training CFD model; generate a training dataset that includes the steady state mixing factors associated with each training steady state mixing configuration, and the calculated mixing quality for each training steady state mixing configuration; train a machine learning model, using the training dataset, to predict mixing qualities for steady state mixing configurations based on steady state mixing factors associated with the steady state mixing configurations; and recommend one or more of a working volume or an impeller speed for a given product based on the trained machine learning model.

BRIEF DESCRIPTION OF THE DRAWINGS

[0009] FIG. 1 illustrates an example steady-state mixing tank in which the systems and methods described herein may be implemented, in some examples.

[0010] FIG. 2 illustrates relationships between various steady state mixing factors used in training a surrogate machine learning model to predict mixing quality, in accordance with some examples described herein.

[0011] FIG. 3 illustrates a flow diagram of an example method of training a surrogate machine learning model to predict mixing quality in a steady-state mixing tank, in accordance with some examples described herein.

substance, and/or other chemical and pharmaceutical properties for each substance involved in the mixing, or any other suitable steady state mixing factors associated with a given steady state mixing configuration in which inlet streams are mixed in a tank.

[0037] A mixing quality may be calculated (block 904) for each steady state mixing configuration using each respective training CFD model. For instance, the mixing quality may be a measure of the standard deviation of trace concentration in the tank.

[0038] A training dataset that includes the steady state mixing factors associated with each training steady state mixing configuration, and the calculated mixing quality for each training steady state mixing configuration may be generated (block 906).

[0039] Using the training dataset, a machine learning model may be trained (block 908) to predict mixing qualities for steady state mixing configurations based on steady state mixing factors associated with the steady state mixing configurations. In some examples, the machine learning model may be a deep learning model.

[0040] In some examples, the method 900 may additionally include applying (block 910) the trained machine learning model to new steady state mixing factors associated with a new steady state mixing configuration; and predicting (block 912) a mixing quality for the new steady state mixing configuration based on applying the trained machine learning model to the steady state mixing factors associated with the new steady state mixing configuration.

[0041] Additionally, in some examples, the method 900 may further include generating at least one testing CFD model for a testing steady state mixing configuration in which inlet streams are mixed in a tank. Like the plurality of training CFD models generated at block 902, the testing CFD model may be generated based on a plurality of steady state mixing factors associated with the testing steady state mixing configuration. A mixing quality may then be calculated for the testing steady state mixing configuration using the testing CFD model. The machine learning model trained at block 908 may then be applied to the steady state mixing factors associated with the testing steady state mixing configuration, and a quality of mixing may be predicted for the testing steady state mixing configuration using the trained machine learning model. The trained machine learning model may then be evaluated based on comparing the mixing quality calculated for the testing steady state mixing configuration using the testing CFD model to the mixing quality predicted for the testing steady state mixing configuration using the trained machine learning model. For instance, the trained machine learning model may be evaluated based on how closely the mixing quality calculated by the testing CFD model for the testing steady state mixing configuration matches the mixing quality predicted by the trained machine learning model for the testing steady state mixing configuration. In some examples the trained machine learning model may be modified based on the evaluation, *e.g.*, if the predicted mixing quality differs from the calculated mixing quality by greater than a threshold amount.

ASPECTS

[0042] Embodiments of the techniques described in the present disclosure may include any number of the following aspects, either alone or combination:

[0043] 1. A method, comprising: generating, by one or more processors, a plurality of training computational fluid dynamic (CFD) models for a plurality of training steady state mixing configurations in which inlet streams are mixed in tanks, wherein each training CFD model is generated based on a plurality of steady state mixing factors associated with each training steady state mixing configuration; calculating, by the one or more processors, a mixing quality for each training steady state mixing configuration using each respective training CFD model; generating, by the one or more processors, a training dataset that includes the steady state

mixing factors associated with each training steady state mixing configuration, and the calculated mixing quality for each training steady state mixing configuration; and training, by the one or more processors, a machine learning model, using the training dataset, to predict mixing qualities for steady state mixing configurations based on steady state mixing factors associated with the steady state mixing configurations.

[0044] 2. The method of aspect 1, further comprising: applying, by the one or more processors, the trained machine learning model to new steady state mixing factors associated with a new steady state mixing configuration; and predicting, by the one or more processors, based on applying the trained machine learning model to the steady state mixing factors associated with the new steady state mixing configuration, a mixing quality for the new steady state mixing configuration.

[0045] 3. The method of any of aspects 1 or 2, wherein the steady state mixing factors include one or more of: tank geometry, stirrer geometry, working volume, inlet configuration, outlet configuration, inlet flow rates for each inlet, outlet flow rates for each outlet, agitation speed, impeller speed, fluid Reynolds number for each substance, and other chemical and pharmaceutical properties for each substance.

[0046] 4. The method of any of aspects 1-3, wherein the mixing quality is a measure of standard deviation of trace concentration in the tank.

[0047] 5. The method of any of aspects 1-4, further comprising: generating, by the one or more processors, a testing computational fluid dynamic (CFD) model for a testing steady state mixing configuration in which inlet streams are mixed in tanks, wherein the testing CFD model is generated based on a plurality of steady state mixing factors associated with the testing steady state mixing configuration; calculating, by the one or more processors, a mixing quality for the testing steady state mixing configuration using the testing CFD model; applying, by the one or more processors, the trained machine learning model to the steady state mixing factors associated with the testing steady state mixing configuration; predicting, by the one or more processors, based on applying the trained machine learning model to the steady state mixing factors associated with the testing steady state mixing configuration, a quality of mixing for the testing steady state mixing configuration; and evaluating, by the one or more processors, the trained machine learning model by comparing the mixing quality calculated for the testing steady state mixing configuration using the testing CFD model and the mixing quality predicted for the testing steady state mixing configuration using the trained machine learning model.

[0048] 6. The method of any of aspects 1-5, wherein the machine learning model is a deep learning model.

[0049] 7. A computer system, comprising: one or more processors; and a non-transitory program memory communicatively coupled to the one or more processors and storing executable instructions that, when executed by the one or more processors, cause the processors to: generate a plurality of training computational fluid dynamic (CFD) models for a plurality of training steady state mixing configurations in which inlet streams are mixed in tanks, wherein each training CFD model is generated based on a plurality of steady state mixing factors associated with each training steady state mixing configuration; calculate a mixing quality for each training steady state mixing configuration using each respective training CFD model; generate a training dataset that includes the steady state mixing factors associated with each training steady state mixing configuration, and the calculated mixing quality for each training steady state mixing configuration; and train a machine learning model, using the training dataset, to predict mixing qualities for steady state mixing configurations based on steady state mixing factors associated with the steady state mixing configurations.

configuration, and the calculated mixing quality for each training steady state mixing configuration; and train a machine learning model, using the training dataset, to predict mixing qualities for steady state mixing configurations based on steady state mixing factors associated with the steady state mixing configurations.

[0058] 16. The non-transitory computer readable storage medium of aspect 15, wherein the computer-readable instructions, when executed by the one or more processors, further cause the processors to: apply the trained machine learning model to new steady state mixing factors associated with a new steady state mixing configuration; and predict, based on applying the trained machine learning model to the steady state mixing factors associated with the new steady state mixing configuration, a mixing quality for the new steady state mixing configuration.

[0059] 17. The non-transitory computer readable storage medium of any of aspects 15 or 16, wherein the steady state mixing factors include one or more of: tank geometry, stirrer geometry, working volume, inlet configuration, outlet configuration, inlet flow rates for each inlet, outlet flow rates for each outlet, agitation speed, impeller speed, fluid Reynolds number for each substance, and other chemical and pharmaceutical properties for each substance.

[0060] 18. The non-transitory computer readable storage medium of any of aspects 15-17, wherein the mixing quality is a measure of standard deviation of trace concentration in the tank.

[0061] 19. The non-transitory computer readable storage medium of any of aspects 15-18, wherein the computer-readable instructions, when executed by the one or more processors, further cause the processors to: generate a testing computational fluid dynamic (CFD) model for a testing steady state mixing configuration in which inlet streams are mixed in tanks, wherein the testing CFD model is generated based on a plurality of steady state mixing factors associated with the testing steady state mixing configuration; calculate a mixing quality for the testing steady state mixing configuration using the testing CFD model; apply the trained machine learning model to the steady state mixing factors associated with the testing steady state mixing configuration; predict, based on applying the trained machine learning model to the steady state mixing factors associated with the testing steady state mixing configuration, a quality of mixing for the testing steady state mixing configuration; and evaluate the trained machine learning model by comparing the mixing quality calculated for the testing steady state mixing configuration using the testing CFD model and the mixing quality predicted for the testing steady state mixing configuration using the trained machine learning model.

[0062] 20. The non-transitory computer readable storage medium of any of aspects 15-19, wherein the machine learning model is a deep learning model.

What is Claimed is:

1. A method, comprising:

generating, by one or more processors, a plurality of training computational fluid dynamic (CFD) models for a plurality of training steady state mixing configurations in which inlet streams are mixed in tanks, wherein each training CFD model is generated based on a plurality of steady state mixing factors associated with each training steady state mixing configuration;

calculating, by the one or more processors, a mixing quality for each training steady state mixing configuration using each respective training CFD model;

generating, by the one or more processors, a training dataset that includes the steady state mixing factors associated with each training steady state mixing configuration, and the calculated mixing quality for each training steady state mixing configuration;

training, by the one or more processors, a machine learning model, using the training dataset, to predict mixing qualities for steady state mixing configurations based on steady state mixing factors associated with the steady state mixing configurations; and

recommending, by the one or more processors, one or more of a working volume or an impeller speed for a given product based on the trained machine learning model.

2. The method of claim 1, further comprising:

applying, by the one or more processors, the trained machine learning model to new steady state mixing factors associated with a new steady state mixing configuration; and

predicting, by the one or more processors, based on applying the trained machine learning model to the steady state mixing factors associated with the new steady state mixing configuration, a mixing quality for the new steady state mixing configuration.

3. The method of claim 1, wherein the steady state mixing factors include one or more of: tank geometry, stirrer geometry, working volume, inlet configuration, outlet configuration, inlet flow rates for each inlet, outlet flow rates for each outlet, agitation speed, impeller speed, fluid Reynolds number for each substance, and other chemical and pharmaceutical properties for each substance.

4. The method of claim 1, wherein the mixing quality is a measure of standard deviation of trace concentration in the tank.

5. The method of claim 1, further comprising:

generating, by the one or more processors, a testing computational fluid dynamic (CFD) model for a testing steady state mixing configuration in which inlet streams are mixed in tanks, wherein the testing CFD model is generated based on a plurality of steady state mixing factors associated with the testing steady state mixing configuration;

calculating, by the one or more processors, a mixing quality for the testing steady state mixing configuration using the testing CFD model;

applying, by the one or more processors, the trained machine learning model to the steady state mixing factors associated with the testing steady state mixing configuration;

predicting, by the one or more processors, based on applying the trained machine learning model to the steady state mixing factors associated with the testing steady state mixing configuration, a quality of mixing for the testing steady state mixing configuration; and

evaluating, by the one or more processors, the trained machine learning model by comparing the mixing quality calculated for the testing steady state mixing configuration using the testing CFD model and the mixing quality predicted for the testing steady state mixing configuration using the trained machine learning model.

6. The method of claim 1, wherein the machine learning model is a deep learning model.

7. A computer system, comprising:

one or more processors; and

a non-transitory program memory communicatively coupled to the one or more processors and storing executable instructions that, when executed by the one or more processors, cause the processors to:

generate a plurality of training computational fluid dynamic (CFD) models for a plurality of training steady state mixing configurations in which inlet streams are mixed in tanks, wherein each training CFD model is generated based on a plurality of steady state mixing factors associated with each training steady state mixing configuration;

calculate a mixing quality for each training steady state mixing configuration using each respective training CFD model;

generate a training dataset that includes the steady state mixing factors associated with each training steady state mixing configuration, and the calculated mixing quality for each training steady state mixing configuration;

train a machine learning model, using the training dataset, to predict mixing qualities for steady state mixing configurations based on steady state mixing factors associated with the steady state mixing configurations; and

recommend one or more of a working volume or an impeller speed for a given product based on the trained machine learning model.

8. The computer system of claim 7, wherein a first set of one or more processors, of the one or more processors, generate the plurality of training computational fluid dynamic (CFD) models, and wherein a second set of one or more processors, of the one or more processors, train the machine learning model.

9. The computer system of claim 7, wherein the executable instructions, when executed by the one or more processors, further cause the processors to:

apply the trained machine learning model to new steady state mixing factors associated with a new steady state mixing configuration; and

predict, based on applying the trained machine learning model to the steady state mixing factors associated with the new steady state mixing configuration, a mixing quality for the new steady state mixing configuration.

10. The computer system of claim 9, wherein a third set of one or more processors, of the one or more processors, apply the trained machine learning model to the new steady state mixing factors associated with the new steady state mixing configuration and predict the mixing quality for the new steady state mixing configuration.

11. The computer system of claim 7, wherein the steady state mixing factors include one or more of: tank geometry, stirrer geometry, working volume, inlet configuration, outlet configuration, inlet flow rates for each inlet, outlet flow rates for each outlet, agitation speed, impeller speed, fluid Reynolds number for each substance, and other chemical and pharmaceutical properties for each substance.

12. The computer system of claim 7, wherein the mixing quality is a measure of standard deviation of trace concentration in the tank.

13. The computer system of claim 7, wherein the executable instructions, when executed by the one or more processors, further cause the processors to:

generate a testing computational fluid dynamic (CFD) model for a testing steady state mixing configuration in which inlet streams are mixed in tanks, wherein the testing CFD model is generated based on a plurality of steady state mixing factors associated with the testing steady state mixing configuration;

calculate a mixing quality for the testing steady state mixing configuration using the testing CFD model;

apply the trained machine learning model to the steady state mixing factors associated with the testing steady state mixing configuration;

predict, based on applying the trained machine learning model to the steady state mixing factors associated with the testing steady state mixing configuration, a quality of mixing for the testing steady state mixing configuration; and

evaluate the trained machine learning model by comparing the mixing quality calculated for the testing steady state mixing configuration using the testing CFD model and the mixing quality predicted for the testing steady state mixing configuration using the trained machine learning model.

14. The computer system of claim 7, wherein the machine learning model is a deep learning model.

15. A non-transitory computer readable storage medium storing computer-readable instructions that, when executed by one or more processors, cause the one or more processors to:

generate a plurality of training computational fluid dynamic (CFD) models for a plurality of training steady state mixing configurations in which inlet streams are mixed in tanks, wherein each training CFD model is generated based on a plurality of steady state mixing factors associated with each training steady state mixing configuration;

calculate a mixing quality for each training steady state mixing configuration using each respective training CFD model;

generate a training dataset that includes the steady state mixing factors associated with each training steady state mixing configuration, and the calculated mixing quality for each training steady state mixing configuration;

train a machine learning model, using the training dataset, to predict mixing qualities for steady state mixing configurations based on steady state mixing factors associated with the steady state mixing configurations; and

recommend one or more of a working volume or an impeller speed for a given product based on the trained machine learning model.

16. The non-transitory computer readable storage medium of claim 15, wherein the computer-readable instructions, when executed by the one or more processors, further cause the processors to:

apply the trained machine learning model to new steady state mixing factors associated with a new steady state mixing configuration; and

predict, based on applying the trained machine learning model to the steady state mixing factors associated with the new steady state mixing configuration, a mixing quality for the new steady state mixing configuration.

17. The non-transitory computer readable storage medium of claim 15, wherein the steady state mixing factors include one or more of: tank geometry, stirrer geometry, working volume, inlet configuration, outlet configuration, inlet flow rates for each inlet, outlet flow rates for each outlet, agitation speed, impeller speed, fluid Reynolds number for each substance, and other chemical and pharmaceutical properties for each substance.

18. The non-transitory computer readable storage medium of claim 15, wherein the mixing quality is a measure of standard deviation of trace concentration in the tank.

19. The non-transitory computer readable storage medium of claim 15, wherein the computer-readable instructions, when executed by the one or more processors, further cause the processors to:

generate a testing computational fluid dynamic (CFD) model for a testing steady state mixing configuration in which inlet streams are mixed in tanks, wherein the testing CFD model is generated based on a plurality of steady state mixing factors associated with the testing steady state mixing configuration;

calculate a mixing quality for the testing steady state mixing configuration using the testing CFD model;

apply the trained machine learning model to the steady state mixing factors associated with the testing steady state mixing configuration;

predict, based on applying the trained machine learning model to the steady state mixing factors associated with the testing steady state mixing configuration, a quality of mixing for the testing steady state mixing configuration; and

evaluate the trained machine learning model by comparing the mixing quality calculated for the testing steady state mixing configuration using the testing CFD model and the mixing quality predicted for the testing steady state mixing configuration using the trained machine learning model.

20. The non-transitory computer readable storage medium of claim 15, wherein the machine learning model is a deep learning model.