

(51) International Patent Classification:
G06F 19/00 (2018.01)(21) International Application Number:
PCT/IB2018/052879(22) International Filing Date:
25 April 2018 (25.04.2018)

(25) Filing Language: English

(26) Publication Language: English

(30) Priority Data:
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(81) Designated States (unless otherwise indicated, for every kind of national protection available): AE, AG, AL, AM, AO, AT, AU, AZ, BA, BB, BG, BH, BN, BR, BW, BY, BZ, CA, CH, CL, CN, CO, CR, CU, CZ, DE, DJ, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IR, IS, JO, JP, KE, KG, KH, KN, KP,

KR, KW, KZ, LA, LC, LK, LR, LS, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PA, PE, PG, PH, PL, PT, QA, RO, RS, RU, RW, SA, SC, SD, SE, SG, SK, SL, SM, ST, SV, SY, TH, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW.

(84) Designated States (unless otherwise indicated, for every kind of regional protection available): ARIPO (BW, GH, GM, KE, LR, LS, MW, MZ, NA, RW, SD, SL, ST, SZ, TZ, UG, ZM, ZW), Eurasian (AM, AZ, BY, KG, KZ, RU, TJ, TM), European (AL, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HR, HU, IE, IS, IT, LT, LU, LV, MC, MK, MT, NL, NO, PL, PT, RO, RS, SE, SI, SK, SM, TR), OAPI (BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, KM, ML, MR, NE, SN, TD, TG).

Declarations under Rule 4.17:

- as to applicant's entitlement to apply for and be granted a patent (Rule 4.17(ii))
- as to the applicant's entitlement to claim the priority of the earlier application (Rule 4.17(iii))

Published:

- without international search report and to be republished upon receipt of that report (Rule 48.2(g))

(54) Title: CHEMICAL PROCESS INTENSIFICATION DESIGN THROUGH MODELING AND ADDITIVE MANUFACTURING

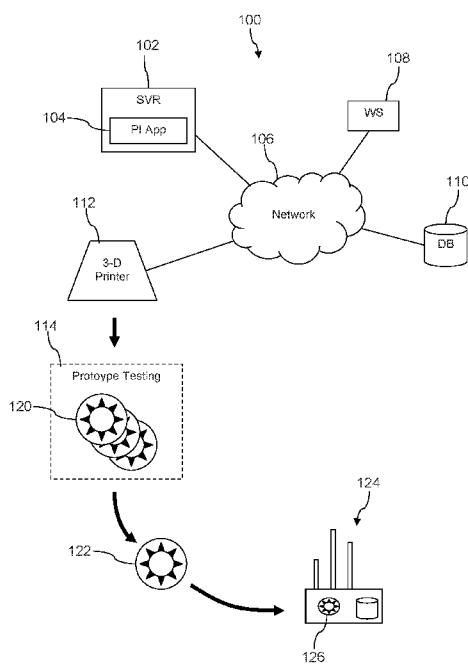


FIG. 1

(57) **Abstract:** A method of chemical process intensification by designing a chemical process component through modeling using dimensionless numbers. The method comprises identifying the inter-relationship between chemical process engineering parameters and structures for subcomponents of the chemical process component, defining a weighting among a plurality of dimensionless numbers associated with a processing function of the subcomponents, simulating a chemical process for each of a plurality of combinations of subcomponent designs to determine, for each combination, a value for each of the plurality of the dimensionless numbers, determining a simulation score for each simulated chemical process based on the plurality of dimensionless numbers determined for that simulated chemical process and based on the defined weighting among the plurality of dimensionless numbers, and selecting a combination of subcomponent designs associated with an extreme simulation scores.

Chemical Process Intensification Design through Modeling and Additive Manufacturing

BACKGROUND

[0001] The concept of 'process intensification' in chemical engineering dates from before the First International Conference on Process Intensification in the Chemical Industry that took place in 1995. An initial definition of 'process intensification' from 1995 as "a strategy for making dramatic reductions in the size of a chemical plant to achieve a given production objective" (Ramshaw 1995) has been deemed too limited and narrow. Process intensification (PI) can be defined as a development or advance of chemical processing or chemical processing equipment that leads to a substantial improvement in some parameter of the total chemical processing system. These parameters may include reduced size of processing equipment, less generation of waste products, less consumption of energy, quicker process cycles, and the like.

SUMMARY

[0002] In an embodiment, a method of designing and testing a chemical process component is disclosed. The method comprises identifying the inter-relationship between different chemical process engineering parameters and structures for subcomponents of the chemical process component, defining a weighting among a plurality of dimensionless numbers associated with a processing function of the subcomponents, simulating a chemical process for each of a plurality of combinations of subcomponent designs by an application executing on a computer system to determine, for each combination, a value for each of the plurality of the dimensionless numbers, and determining a simulation score by the application for each simulated chemical process based on the plurality of dimensionless numbers determined for that simulated chemical process and based on the defined weighting among the plurality of dimensionless numbers. The method further comprises selecting a plurality of the combinations of subcomponent designs based on the simulation scores, building a prototype of the chemical process component using a 3-dimensional printer for each of the selected combinations of subcomponent designs, testing each of the prototypes of the chemical process component, and selecting one of the prototypes based on production criteria.

[0003] In another embodiment, a method of building a chemical process component and using the component in a chemical processing plant is disclosed. The method

comprises identifying the inter-relationship between different chemical process engineering parameters and structures for subcomponents of the chemical process component, defining a weighting among a plurality of dimensionless numbers associated with a processing function of the subcomponents, simulating a chemical process for each of a plurality of combinations of subcomponent designs by a computer application executing on a computer to determine, for each combination, a value for each of the plurality of the dimensionless numbers, and determining a simulation score for each simulated chemical process by the application based on the plurality of dimensionless numbers determined for that simulated chemical process and based on the defined weighting among the plurality of dimensionless numbers. The method further comprises selecting a combination of subcomponent designs based on simulation scores, building a chemical process component according to the selected combination of subcomponent designs, installing the chemical process component in a chemical processing plant, and producing a chemical product by the chemical processing plant.

[0004] In yet another embodiment, a method of chemical process intensification by designing a chemical process component through modeling using dimensionless numbers is disclosed. The method comprises identifying the inter-relationship between different chemical process engineering parameters and structures for subcomponents of the chemical process component, defining a weighting among a plurality of dimensionless numbers associated with a processing function of the subcomponents, simulating a chemical process for each of a plurality of combinations of subcomponent designs by an application executing on a computer system to determine, for each combination, a value for each of the plurality of the dimensionless numbers, determining a simulation score for each simulated chemical process by the application based on the plurality of dimensionless numbers determined for that simulated chemical process and based on the defined weighting among the plurality of dimensionless numbers, and selecting a combination of subcomponent designs based on each selected subcomponent design having a maximum simulation score or having a minimum simulation score.

[0005] These and other features will be more clearly understood from the following detailed description taken in conjunction with the accompanying drawings and claims.

BRIEF DESCRIPTION OF THE DRAWINGS

[0006] For a more complete understanding of the present disclosure, reference is now made to the following brief description, taken in connection with the accompanying drawings and detailed description, wherein like reference numerals represent like parts.

[0007] FIG. 1 is an illustration of a system according to an embodiment of the disclosure.

[0008] FIG. 2A, FIG. 2B, and FIG. 2C illustrate an exemplary stirrer component designed using a system according to an embodiment of the disclosure.

[0009] FIG. 3A, FIG. 3B, FIG. 3C, FIG. 3D, FIG. 3E, FIG. 3F, FIG. 3G, and FIG. 3H illustrate an exemplary catalyst pack/separator component designed using a system according to an embodiment of the disclosure.

[0010] FIG. 4A and FIG. 4B is a flow chart of a method according to an embodiment of the disclosure.

[0011] FIG. 5 is a block diagram of a computer system according to an embodiment of the disclosure.

DETAILED DESCRIPTION

[0012] It should be understood at the outset that although illustrative implementations of one or more embodiments are illustrated below, the disclosed systems and methods may be implemented using any number of techniques, whether currently known or not yet in existence. The disclosure should in no way be limited to the illustrative implementations, drawings, and techniques illustrated below, but may be modified within the scope of the appended claims along with their full scope of equivalents.

[0013] The conventional process for optimization of chemical process engineering unit operations and process intensification equipment typically takes three or more years. In extreme cases, the conventional process may take ten years or more. Additionally, this conventional process, involving intuitive and craft knowledge, is constrained to examining conventional structures, constrained to “inside the box” thinking about structures, because the range of potential structures of components is artificially constrained by considerations of the ease of machining and building prototypes. Said in other words, in the conventional process, component designs that are difficult to build – but which may have produced brilliant chemical processing results – are excluded from consideration. The conventional process of building chemical processing components is an iterative process that involves the steps of (1) generating a large number of alternatives by an ad hoc, craft-like process (e.g., as many as 200 to

300 alternatives), (2) modeling the alternatives with engineering tools, (3) based on results of modeling selecting a single design alternative for prototyping and then building the prototype, (4) testing the prototype to capture chemical process target parameters, and (5) reiterating steps 1-4 based on the captured target parameters. This conventional process may be referred to as a test through modeling which proceeds by blind trial and error, largely unguided by analysis. This conventional process can be analogized to an "Edison-ian" design process, where all known alternatives are blindly considered and modeled. These limitations of the conventional approach result in both lost revenue opportunities from the delay of process optimization and also greater investment costs in the lengthy optimization process. But more importantly, the conventional approach leads to shortfalls in final equipment design, shortfalls of product for end use customers, and delay in bringing useful new chemicals to market.

[0014] At a summary level, the disclosed new process comprises steps of (1) proposing structures for sub-components of the chemical processing component; (2) designing the proposed structures using a computer algorithm that optimizes each structure based on achieving target values of dimensionless numbers determined by simulation of the subject structure (unlike human design, this computer algorithm is a quasi-continuous process – for example, instead of simulating tens of variations in the design of the basic structure, as in conventional processes, rather tens of thousands, hundreds of thousands of slight variations of the design of sub-components of the basic structures are simulated to find the specific design that optimizes that dimensionless number goal); (3) the structures of the sub-components are combined as an aggregate component and simulated; (4) a selected set of the simulated sub-components (selected based on preferred performance in respect of the dimensionless numbers determined during simulation) are built using additive manufacturing (AM) processes; and (5) the selected set of built sub-components along with final structures are built using an additive manufacturing process and tested in a chemical processing system, at a demonstration/pilot scale, to screen and arrive quickly at the most optimal structure. The steps 1-5 may be repeated to achieve a desired end result, but often the result of the first pass through this process achieves success. The finalized design is then built to provide the production chemical process component using an additive manufacturing process or a conventional machining process may be used to build the finalized design.

[0015] Additive manufacturing processes (sometimes referred to as 3-D printing) offers the design freedom to build chemical processing structures of almost any form, even designs which are not feasible with traditional methods such as by machining. The choice of material could be polymers, resins, plastics, metals, ceramics, or other materials based on the stage of chemical engineering process development viz., lab scale, pilot scale or bench scale. Additionally, using additive manufacturing processes enables concurrent building of alternative prototypes (using separate advanced manufacturing machines or 3-D printers) so prototype testing and/or simulation may proceed in parallel for multiple alternative prototype designs. Conventional machining of prototypes does not typically support concurrent machining of multiple prototypes, because of resource constraints on machines and technicians. Additive manufacturing refers to processes that can synthesize a three-dimensional object by forming successive layers of material under computer control. In some contexts, additive manufacturing may be referred to as advanced manufacturing.

[0016] Additive manufacturing processes may comprise vat photo-polymerization, material extrusion, material jetting, binder jetting, powder bed fusion, direct energy deposition, and sheet lamination. Vat photo-polymerization additive manufacturing may comprise stereo-lithography, digital light processing, and/or continuous digital light processing technologies. Material extrusion additive manufacturing may comprise fused deposition modeling processing technologies. Material jetting additive manufacturing may comprise material jetting, nanoparticle jetting, and/or drop on demand processing technologies. Powder bed fusion additive manufacturing may comprise multi jet fusion, selective laser sintering, direct metal laser sintering selective laser melting, and electron beam melting processing technologies. Direct energy deposition additive manufacturing may comprise laser engineering new shape and/or electron beam additive manufacturing processing technologies. Sheet lamination additive manufacturing may comprise laminated object manufacturing processing technologies. The additive manufacturing technology area is being actively extended, and the present disclosure contemplates using other additive manufacturing technologies as they evolve and are commercialized for the chemical process intensification design methods taught herein.

[0017] The first and second steps in the new process taught herein may be repeated multiple times or iterated multiple times. The first step may include proposing different trade-off rules for competing dimensionless numbers, which lead to different results in

the second step. Additionally, the design of sub-component structures involves varying the design of the subject subcomponent structure while simulating the aggregate component (with the subcomponent whose design is being varied) using controlled, non-varied design for the other subcomponents.

[0018] This new process has a stepwise sequence where the results of one step sets up the initial starting point for the next step in the process. This process, as mentioned above, enables reaching designs that are not typically reached by the conventional process if at all. It is thought that the automated designing using dimensionless numbers in a process of simulating or modeling a very great number of slight variations of the sub-components of the overall design, where the range of the variation of the design is not artificially constrained by conventional heuristic: "the end design has to look pretty much like what we have done before and/or an item that we can feasibly manufacture." The new process taught herein may be referred to as an "Einstein-ian" approach, as it is based on analysis rather than blind trial and error. The new process may be referred to as an "optimization approach through modeling employing dimensionless numbers and additive manufacturing."

[0019] It happens that, given a specific trade-off of rules for competing dimensionless numbers (e.g., changing the component by change A changes dimensionless number 1 in a preferred sense but changes dimensionless number 2 in an undesirable sense) the process can arrive at metastable designs that optimize for the subject recipe of dimensionless numbers but may not be optimized for the end chemical process engineering parameters. This eventuality is provided for by working through several alternative recipes or trade-off rules for competing dimensionless numbers and modeling or testing the metastable designs that flow from these alternative recipes. All possibilities of metastable designs can be 3D printed for quick prototype testing to arrive at the best design.

[0020] Turning now to FIG. 1, a system 100 is described. In an embodiment, system 100 comprises a computer system 102 executing a process intensification (PI) application 104, a communication network 106, a workstation 108, a data store 110, and a 3-dimensional (3-D) printer 112. The system 100 may be used to design and build by the 3-D printer 112 a plurality of prototypes of a chemical process component 120. It is understood that the 3-D printer 112 may use any additive manufacturing process, for example any of vat photo-polymerization, material extrusion, material jetting, binder jetting, powder bed fusion, direct energy deposition, and sheet lamination.

The prototypes 120 may undergo prototype testing 114 in an actual chemical process at a lab scale or a pilot scale. Alternatively, the prototypes 120 may undergo simulation. A preferred design 122 from among the several prototypes 120 may be selected for being built at a full-production scale component 126 for incorporation in a chemical production plant 124. It is noted that the representation of a chemical process component 120, 122, 126 in FIG. 1 is not intended to represent an actual specific component but rather to suggest any component. The chemical process component 120 may be a separator component, a mixing component, a reactor component, a heat transfer component, a flow enhancement component, a sampler component, a mass transfer component, a hydrodynamic/flow dynamic component, a thermodynamic component, or a mechanical process component. A separate component may be a distillation column, a stripping column, an extraction column, a membrane, a chromatographic component, or a filtration component. The mixing component may be a static mixer or a stirrer. The reactor component may be a batch reactor, a continuous stirred tank reactor, a buzz loop reactor, a plug flow reactor, or a micro-reactor. The heat transfer component may be a heat exchanger or a finned heat intensification component. The mass transfer component may be a liquid-liquid/VLE extraction component, a vapor compression evaporator, a crystallizer, a spray dryer, an adsorption component, or an absorption component. The hydrodynamic/flow dynamic component may be a pump, a flow pipe, a flow conduit, a vortex generator, a turbulent mixer, or an extrusion component. The thermodynamic component may be a gas liquefaction component, a cryogenic component, or a refrigeration component. The mechanical process component may be a solid transportation component, a crushing component, a milling component, a pulverization component, a palletization component, a screening component, or a sieving component. The chemical process component 120 may be a combined component, for example a component that functions both as a separator component and as a reactor component (e.g., reactive separation). Other combined component examples are a HEX reactor (heat exchanger reactor), a divided wall column, micro-channel reactors, millisecond/short residence time reactors.

[0021] The system may comprise a plurality of 3-D printers 112, for example to promote printing different prototypes 120 concurrently using different ones of the plurality of 3-D printers 112. While represented in FIG. 1 and discussed herein as a single application, the capabilities and actions attributed to the PI application 104, in an embodiment, may be delivered by a plurality of separate applications executing on the

same computer or on different computers. It is understood that the computer system 102 may be implemented as a single computer or by a plurality of computers, for example by a plurality of servers. Computer systems are discussed further hereinafter. The data store 110 may be implemented by one or more physical disk drives. Alternatively, the data store 110 may be implemented as one or more solid state memories. In an embodiment, the PI application 104 may be executed in a cloud computing environment, and the data store 110 may be provided by memory resources in the cloud computing environment. The network 106 comprises one or more private networks, one or more public networks, or a combination thereof.

[0022] A technician or engineer, hereinafter referred to as a designer, may use the workstation 108 to access a user interface (UI) extended by the PI application 104. The UI allows the designer to use the PI application 104 to design and build prototypes 120. The design process comprises identifying a component structure by defining sub-component structures. For example, a distillation column/separator component structure may comprise an enclosure sub-component, a plurality of sheet sub-components that are parallel with the axis of the enclosure, spacer sub components that are transverse to the axis of the enclosure, and catalyst pack sub-components that are placed between the sheets.

[0023] The design process further comprises designing the sub-component structures using a computer algorithm of the PI application 104 that optimizes each sub-component structure based on achieving target values of dimensionless numbers associated with the overall chemical process provided by the component. The target values of the dimensionless numbers may be determined based on trade-offs between antagonistic dimensionless numbers (e.g., in the given chemical process, adapting structures to increase a first dimensionless number may entail the decrease of a second dimensionless number). These trade-offs may be referred to as recipes of dimensionless numbers, prioritization among dimensionless numbers, or weightings among dimensionless numbers, and the structures may be designed for each of a plurality of different recipes of the dimensionless numbers.

[0024] Dimensionless numbers are attributes of physical systems that have no dimensions and are used to describe the ratios of various physical quantities. An example dimensionless number is the Reynolds Number which is a measure of laminar fluid flow or a measure of turbulence of a fluid flow. Other dimensionless numbers are identified below, but it is understood that other dimensionless numbers that are not

explicitly identified here may be used in the system 100 for designing, prototyping, building, and performing chemical processing.

Table 1

Biot Number (Bi)	Ratio of the internal thermal resistance of a solid to the boundary layer thermal resistance
Coefficient of friction	Dimensionless surface shear stress
Drag Coefficient	Ratio of gravitational force to inertial force used in free settling velocities and resistance to flow
Euler Number	Ratio of pressure force to inertial force
Fourier Number	Ratio of the heat conduction rate to the rate of thermal energy storage in a solid
Friction Factor	Dimensionless pressure drop for internal flow
Gratz Number	Ratio of the thermal capacity to convective heat transfer
Colburn j Factor	Dimensionless heat transfer coefficient
Lewis Number	Ratio of thermal and mass diffusivities
Mach Number	Velocity divided by the speed of sound
Nusselt Number	Dimensionless temperature gradient at the surface
Peclet Number	Dimensionless independent heat transfer parameter
Mass Transfer Peclet Number	Dimensionless independent mass transfer parameter
Prandtl Number	Ratio of momentum and thermal diffusivities
Rayleigh number	Used in heat transfer and free convection calculations
Reynolds Number	Ratio of the inertial and viscous forces
Schmidt Number	Ratio of the momentum and mass diffusivities
Sherwood Number	Dimensionless concentration gradient at the surface
Stanton Number	Modified Nusselt number
Mass Transfer Stanton Number	Modified Sherwood number

[0025] For each candidate recipe of dimensionless numbers for a given component design, the PI application 104 simulates the designs of the sub-components, altering dimensions and features of each sub-component through a range of variation to

converge on an optimal design of the sub-components. In an embodiment, a range of variation of design dimensions and characteristics may be partitioned into a relatively small number of equally distributed dimension or characteristic values. A design associated with each of the combinations of these equally distributed dimension or characteristic values may be simulated to determine a sensitivity of the dimensionless number results at the operating point of the designs. The sensitivity values thus determined may be used to partition the range of variation of design dimensions and characteristics into a considerably larger number of non-equally distributed dimensions or characteristic values but rather distributed according to local sensitivity. So, for example, a portion of the range of a dimension that has higher sensitivity may be allocated more variations to be simulated (e.g., the delta between each different design candidate is smaller) than a different portion of the range of the dimension that has a lower sensitivity which may be allocated fewer variations to be simulated (e.g., the delta between each different design candidate is larger). This principle of simulating a number of different designs with variations distributed as described above may be referred to as sensitivity distribution based automated design.

[0026] The results of the simulations of the many automatically varied designs are evaluated according to the dimensionless number rules or recipes (e.g., tradeoff weightings) to determine an optimal design. Such an optimal design may be determined as the design which achieves a maximum sum of weighted dimensionless number results, using the recipe of dimensionless numbers to determine the weighting. Alternatively, in an embodiment, the optimal design may be determined as the design that achieves a minimum sum of weighted dimensionless number results. This optimal design may be referred to as a local extreme value of a sum of the dimensionless numbers.

[0027] The local extreme value of the dimensionless numbers associated with the optimal designs may be compared to each other, and some of these optimal designs associated with local extreme values are then build using the 3-D printer 112. As used here, it is understood "optimal design" may not refer to the best design over-all but rather the best design given the associated weighting or tradeoff rules for the dimensionless numbers. The 3-D printer 112 can additively manufacture the component in a variety of materials including but not limited to polymers, resins, plastics, metal, aluminum, steel, stainless steel, ceramic, or other materials. Additively manufacturing the different designs of the chemical processing component may

promote building and testing designs which would be impracticable for prototyping in a traditional machining process. This can lead to highly optimized designs which would have been overlooked by the conventional design and prototyping process. Additionally, some of the mean values of the dimensionless numbers located between the local extreme values may be selected and built using the 3-D printer 112.

[0028] Each of the additively manufactured prototypes 120 of the chemical processing component is tested in an actual chemical process, for example in a laboratory setting, in a demonstration scale setting, in a pilot scale setting, and/or in a commercial scale setting. The testing of the prototypes 120 may be performed in parallel. The prototype testing is instrumented to determine physical parameters of the chemical processing such as waste produced, product produced, energy consumed, time consumed, and the like. The prototype 122 that exhibits the best aggregate performance in terms of the physical parameters can be selected as the final component for installation as the component 126 actually deployed in the chemical production plant 124.

[0029] Turning now to FIG. 2A, FIG. 2B, and FIG. 2C, an exemplary stirrer component 150 is described. The stirrer component 150 may be used in a chemical process to stir a mixture of liquids and/or particulate matter to increase the uniformity of distribution of different materials in the mixture. The design was arrived at using the system 100 described further above. The stirrer 150 comprises a first blade 152A and a second blade 152B each coupled to a shaft 153. The first blade 152A is one of four blades aligned in a first plane transverse to the stirrer 150 and attached to the shaft 153. The second blade 152B is one of four blades aligned in a second plane transverse to the stirrer 150 and attached to the shaft 153. The alignment of the blades 152A, 152B are offset angularly with reference to the shaft 153 of the stirrer 150, as best seen in FIG. 2B. A face of the blades 152 comprise a first zig-zag ridge 154 and a second zig-zag ridge 156. The structure of the stirrer component 150, using the system 100 above to design and prototype, was found to both provide optimal stirring as well as low energy input. The zig-zag ridges 154, 156 were found to reduce the energy input to turn the stirrer 150.

[0030] Turning now to FIG. 3A, FIG. 3B, FIG. 3C, FIG. 3D, FIG. 3E, FIG. 3F, FIG. 3G, and FIG. 3H an exemplary catalyst pack/separator component 200 is described. The catalyst pack/separator component 200 may be used in a chemical process to catalyze a reaction among chemical precursors to synthesize a desired compound from

the chemical precursors and to separate the desired compound from waste products. In a particular example, the catalyst pack/separator component 200 may be used to synthesize bisphenol A (BPA) from phenol and acetone precursors. The design of the catalyst pack/separator component 200 was arrived at using the system 100 described further above.

[0031] In an embodiment, the catalyst pack/separator component 200 comprises a housing 204 which is filled with a catalyst assembly 202. In an embodiment, the catalyst pack/separator component 200 comprises a top cap (not shown) that has inlets to admit chemical precursors and a bottom cap (not shown) that has one or more inlets and/or outlets. For example, in an embodiment, the bottom cap has an inlet for nitrogen gas and an outlet for BPA. In an embodiment, the housing 204 may comprise one or more outlets (not shown) between the top and the bottom to exhaust effluent waste products. In an embodiment, the interior wall of the housing 204 comprises helical grooves 206. The catalyst assembly 202 comprises a plurality of plates 212 retained in position by a plurality of disks 210. In an embodiment, the housing is about 100 mm long and about 50 mm in diameter, the disks 210 are placed about 15 mm apart from each other and retain the plates 212 with an about 2.5 mm gap between the plates 212. The plates 212 are oriented substantially parallel to an axis 208, and the disks 210 are oriented substantially perpendicular to the axis 208. An end 204a of the housing 204 may be at a lower end of the component 200, and an end 204b of the housing 204 may be at an upper end of the component 200. When in use, the component 200 may be oriented so the axis 208 is substantially vertical. It is understood that dimensions other than those given in this example for the various components of the catalyst pack/separator component 200 are contemplated by the present disclosure. Also, it is understood that the dimensions of the catalyst pack/separator component 200 may be scaled up to larger sizes, for example up to 10 times scale, up to 15 times scale, up to 20 times scale, up to 25 times scale, up to 30 times scale, up to 35 times scale, or up to 40 times scale. Said in other words, the scale of the catalyst pack/separator component 200 illustrated in FIG. 3 may be a pilot scale embodiment of the design.

[0032] A plurality of mini-bales 214 may be assembled into a plurality of the disks 210. In an embodiment, the mini-bales 214 enclose or contain catalyst and are hexagonal in cross-section. Catalyst packs 232 may enclose catalyst pellets, for example within a fabric enclosure similar to a pillow shell. A catalyst pack 232 may be retained within a bale 230, because the catalyst pellets may swell up to about 100% in

volume in use. In an embodiment, the catalyst may be spherical pellets of ion exchange resin (IER) but in different chemical reaction processes, different catalysts may be used. Bales 230 may be inserted between adjacent plates 212 in the catalyst pack/separator component 200. In an embodiment, three bales 230 are inserted into spaces between four plates 212.

[0033] The plates 212 may feature a corrugated shape provided by grooves 222 in the plates 212. The plates 212 may feature a plurality of holes. As best seen in FIG. 3D and FIG. 3E, the numbers of holes may vary from a top of the catalyst pack/separator component 200 to the bottom (from proximate the end 204b of the housing 204 to the proximate end 204a of the housing 204), for example from six holes 220a per horizontal row at a top of the plate 212, to seven holes 220b per horizontal row in the middle of the plate 212, to eight holes 220c per horizontal row at a bottom of the plate 212. The flow of chemical precursors into the top of the catalyst pack/separator component 200 is encouraged to flow in particular patterns by the holes 220 and the grooves 222 of the plates 212, by the helical grooves 206 of the housing 204, and by the vertices of the edges of the hexagonal mini-bales 214, and thereby to engage optimally with the mini-bales 214 and the bales 230 to complete the desired chemical reaction.

[0034] The disks 210 of the catalyst pack/separator component 200 act as distributor plates that, with the plates 212, establish well defined flow paths within the component 200 to promote desired and controlled hydrodynamics. The corrugations formed by the grooves 222 of the plates 212 are aligned at strategic angles to enable increased mass and heat transfer between a gas and liquid phase within the component 200. The bales 230 are sandwiched between the plates 212 to create open channels that minimize a pressure drop within the component 200. The frequent crisscrossing of the corrugations established by grooves 222 of the plates 212 is proportional to the Gas Sherwood dimensionless number (ShG). The designed increase of corners and/or vertices established by bales 230 and mini-bales 214 promote improved reaction kinematics. The by-passing liquid through open channels provides improved contact with the gas phase resulting in increased mass transport. The catalyst pack/separator component 200 was designed based on analysis of Reynolds number, Peclet number, Schmidt number, Nusselt number, and Sherwood number and optimizing among these dimensionless numbers according to a pre-defined balance criteria by the process described further herein.

[0035] Turning now to FIG. 4A and FIG. 4B, a method 300 is described. At block 302, identify structures for subcomponents of the chemical process component. The chemical process component may be a separator component, a distillation component, a stirrer component, a mixer component, a sampler component, a reactor component, a heat exchanger component, a flow enhancement component, or other component. The component may be a combined component, for example a combined separator and reactor component. The processing of block 302 may comprise identifying the inter-relationship between different chemical process engineering parameters and structures for subcomponents of the chemical process component.

[0036] At block 304, define a weighting among a plurality of dimensionless numbers associated with a processing function of the subcomponents. The dimensionless numbers may comprise at least one associated with a heat transfer chemical engineering process parameter, a mass transfer chemical engineering process parameter, a reaction kinetics chemical engineering process parameter, or a hydrodynamics chemical engineering process parameter. The dimensionless numbers may comprise two or more of a Reynold number, a Peclet number, a Schmidt number, a Nusselt number, a Sherwood number, or a Graetz number. The dimensionless numbers may comprise other dimensionless numbers. The weighting may be coefficients to be multiplied with the dimensionless numbers. The weighting may define coefficients in a simulation score defined as a sum of weighted values of dimensionless numbers. For example, the simulation score may have the form of:

$$\text{Simulation Score} = \sum c_i \times DN_i$$

where the simulation score is the sum of i-number of products, the i-th product being determined as the multiplication of an i-th coefficient c_i or weighting value with an i-th dimensionless number DN_i . A weighting of n-number of dimensionless numbers may be given as a vector of n-number of coefficients ($c_1, c_2, \dots, c_n$). The definition of the weighting of dimensionless numbers may be input by a designer using the user interface of the process intensification application accessed using the workstation 108.

[0037] At block 306, a process intensification and/or chemical process optimization application executing on a computer system simulates a chemical process for each of a plurality of combinations of subcomponent designs to determine, for each combination, a value for each of the plurality of the dimensionless numbers. The process intensification application may automatically generate the different combinations of subcomponent designs, for example to cover a range of possible design alternatives.

For example, the process intensification application may generate 20 different designs that feature varying angles of a surface groove between a maximum angle value and a minimum angle value. The process intensification application may generate 30 different designs that feature varying diameter holes. The combination of all the different angles and all the different hole diameters may comprise about 20 x 30 (e.g., 600) unique combinations of designs. In an embodiment, more than 1,000 different designs may be simulated. In an embodiment, more than 10,000 different designs may be simulated. In an embodiment, more than 50,000 different designs may be simulated. In an embodiment, more than 200,000 different designs may be simulated. The designs may vary from each other by one or more of dimensions of sub-component features, geometry of sub-component features, angles of sub-component features, or other qualities.

[0038] In an embodiment, the process intensification application may perform simulation of many different designs concurrently in different threads of execution or on different processors of a computer system. The distribution of different designs (e.g., the change of value of the subject feature from design to design) may be determined to be uniform. Alternatively, the distribution of different designs may be determined according to an analysis of sensitivity of the combinations of subcomponent designs to variation of a feature dimension or characteristic at a given point (e.g., the distribution of design alternatives may not be uniform but may include more design alternatives clustered around a dimensional value that exhibits higher sensitivity in terms of one or more of the dimensionless numbers).

[0039] At block 308, the process intensification application determines a simulation score for each simulated chemical process based on the values of the plurality of dimensionless numbers determined for that simulated chemical process and based on the defined weighting among the plurality of dimensionless numbers. The processing of block 308 may be performed multiple times using different defined weightings among the values of dimensionless numbers determined during simulation.

[0040] At block 310, the process intensification application selects a plurality of the combinations of subcomponent designs based on the simulation scores. The processing at block 310 may comprise selecting a combination of subcomponent designs based on each selected subcomponent design having a maximum simulation score or having a minimum simulation score. For example, the process intensification application may select combinations of subcomponent designs that correspond to a

mathematical inflection point in a series of simulation scores (e.g., a local maximum or a local minimum of the range of simulation scores associated with a given predefined weighting of dimensionless numbers). In an embodiment, a plurality of combinations of subcomponent designs may be selected for a single predefined weighting of dimensionless numbers (e.g., each inflection point or local extreme value of the simulation scores associated with the single predefined weighting of dimensionless numbers). Alternatively, a single combination of subcomponent designs may be selected for a single predefined weighting of dimensionless numbers. The selection of block 310 may select only a single combination subcomponent designs from among a plurality of different predefined weighting of dimensionless numbers, based on the simulation scores. For example, the selection of block 310 may select five of the combinations of subcomponent designs.

[0041] At block 312, a 3-dimensional printer builds a prototype of the chemical process component under control of the process intensification application for each of the selected combinations of subcomponent designs. In an embodiment, multiple prototypes are selected to be tested based on simulation scores and built by multiple 3-dimensional printers executing concurrently. It is understood that any additive manufacturing process may be employed to build the prototypes and hence to perform the processing of block 312. At block 314, test each of the prototypes of the chemical process component. This testing may be referred to as a pilot test. When multiple different prototypes are built, the testing of the several prototypes may be conducted concurrently. In an embodiment, the prototypes may be evaluated using simulation. At block 316, selecting one of the prototypes based on production criteria. The production criteria can be one or more of a size of the chemical process component, the product output, a waste output, or an energy consumption involved in the prototype testing. In an embodiment, waste outputs may comprise greenhouse gas emissions, slurry, etc. In an embodiment, energy consumption may comprise heat energy, electrical energy, chemical energy, etc.

[0042] At block 318, build a chemical process component according to the selected combination of subcomponent designs. At block 320, install the chemical process component in a chemical processing plant. At block 322, produce a chemical product by the chemical processing plant

[0043] FIG. 5 illustrates a computer system 380 suitable for implementing one or more embodiments disclosed herein. The computer system 380 includes a processor

382 (which may be referred to as a central processor unit or CPU) that is in communication with memory devices including secondary storage 384, read only memory (ROM) 386, random access memory (RAM) 388, input/output (I/O) devices 390, and network connectivity devices 392. The processor 382 may be implemented as one or more CPU chips.

[0044] It is understood that by programming and/or loading executable instructions onto the computer system 380, at least one of the CPU 382, the RAM 388, and the ROM 386 are changed, transforming the computer system 380 in part into a particular machine or apparatus having the novel functionality taught by the present disclosure. It is fundamental to the electrical engineering and software engineering arts that functionality that can be implemented by loading executable software into a computer can be converted to a hardware implementation by well-known design rules. Decisions between implementing a concept in software versus hardware typically hinge on considerations of stability of the design and numbers of units to be produced rather than any issues involved in translating from the software domain to the hardware domain. Generally, a design that is still subject to frequent change may be preferred to be implemented in software, because re-spinning a hardware implementation is more expensive than re-spinning a software design. Generally, a design that is stable that will be produced in large volume may be preferred to be implemented in hardware, for example in an application specific integrated circuit (ASIC), because for large production runs the hardware implementation may be less expensive than the software implementation. Often a design may be developed and tested in a software form and later transformed, by well-known design rules, to an equivalent hardware implementation in an application specific integrated circuit that hardwires the instructions of the software. In the same manner as a machine controlled by a new ASIC is a particular machine or apparatus, likewise a computer that has been programmed and/or loaded with executable instructions may be viewed as a particular machine or apparatus.

[0045] Additionally, after the system 380 is turned on or booted, the CPU 382 may execute a computer program or application. For example, the CPU 382 may execute software or firmware stored in the ROM 386 or stored in the RAM 388. In some cases, on boot and/or when the application is initiated, the CPU 382 may copy the application or portions of the application from the secondary storage 384 to the RAM 388 or to memory space within the CPU 382 itself, and the CPU 382 may then execute

instructions that the application is comprised of. In some cases, the CPU 382 may copy the application or portions of the application from memory accessed via the network connectivity devices 392 or via the I/O devices 390 to the RAM 388 or to memory space within the CPU 382, and the CPU 382 may then execute instructions that the application is comprised of. During execution, an application may load instructions into the CPU 382, for example load some of the instructions of the application into a cache of the CPU 382. In some contexts, an application that is executed may be said to configure the CPU 382 to do something, e.g., to configure the CPU 382 to perform the function or functions promoted by the subject application. When the CPU 382 is configured in this way by the application, the CPU 382 becomes a specific purpose computer or a specific purpose machine.

[0046] The secondary storage 384 is typically comprised of one or more disk drives or tape drives and is used for non-volatile storage of data and as an over-flow data storage device if RAM 388 is not large enough to hold all working data. Secondary storage 384 may be used to store programs which are loaded into RAM 388 when such programs are selected for execution. The ROM 386 is used to store instructions and perhaps data which are read during program execution. ROM 386 is a non-volatile memory device which typically has a small memory capacity relative to the larger memory capacity of secondary storage 384. The RAM 388 is used to store volatile data and perhaps to store instructions. Access to both ROM 386 and RAM 388 is typically faster than to secondary storage 384. The secondary storage 384, the RAM 388, and/or the ROM 386 may be referred to in some contexts as computer readable storage media and/or non-transitory computer readable media.

[0047] I/O devices 390 may include printers, video monitors, liquid crystal displays (LCDs), touch screen displays, keyboards, keypads, switches, dials, mice, track balls, voice recognizers, card readers, paper tape readers, or other well-known input devices.

[0048] The network connectivity devices 392 may take the form of modems, modem banks, Ethernet cards, universal serial bus (USB) interface cards, serial interfaces, token ring cards, fiber distributed data interface (FDDI) cards, wireless local area network (WLAN) cards, radio transceiver cards that promote radio communications using protocols such as code division multiple access (CDMA), global system for mobile communications (GSM), long-term evolution (LTE), worldwide interoperability for microwave access (WiMAX), near field communications (NFC), radio frequency identity (RFID), and/or other air interface protocol radio transceiver cards, and other well-known

network devices. These network connectivity devices 392 may enable the processor 382 to communicate with the Internet or one or more intranets. With such a network connection, it is contemplated that the processor 382 might receive information from the network, or might output information to the network in the course of performing the above-described method steps. Such information, which is often represented as a sequence of instructions to be executed using processor 382, may be received from and outputted to the network, for example, in the form of a computer data signal embodied in a carrier wave.

[0049] Such information, which may include data or instructions to be executed using processor 382 for example, may be received from and outputted to the network, for example, in the form of a computer data baseband signal or signal embodied in a carrier wave. The baseband signal or signal embedded in the carrier wave, or other types of signals currently used or hereafter developed, may be generated according to several methods well-known to one skilled in the art. The baseband signal and/or signal embedded in the carrier wave may be referred to in some contexts as a transitory signal.

[0050] The processor 382 executes instructions, codes, computer programs, scripts which it accesses from hard disk, floppy disk, optical disk (these various disk based systems may all be considered secondary storage 384), flash drive, ROM 386, RAM 388, or the network connectivity devices 392. While only one processor 382 is shown, multiple processors may be present. Thus, while instructions may be discussed as executed by a processor, the instructions may be executed simultaneously, serially, or otherwise executed by one or multiple processors. Instructions, codes, computer programs, scripts, and/or data that may be accessed from the secondary storage 384, for example, hard drives, floppy disks, optical disks, and/or other device, the ROM 386, and/or the RAM 388 may be referred to in some contexts as non-transitory instructions and/or non-transitory information.

[0051] In an embodiment, the computer system 380 may comprise two or more computers in communication with each other that collaborate to perform a task. For example, but not by way of limitation, an application may be partitioned in such a way as to permit concurrent and/or parallel processing of the instructions of the application. Alternatively, the data processed by the application may be partitioned in such a way as to permit concurrent and/or parallel processing of different portions of a data set by the two or more computers. In an embodiment, virtualization software may be employed by

the computer system 380 to provide the functionality of a number of servers that is not directly bound to the number of computers in the computer system 380. For example, virtualization software may provide twenty virtual servers on four physical computers. In an embodiment, the functionality disclosed above may be provided by executing the application and/or applications in a cloud computing environment. Cloud computing may comprise providing computing services via a network connection using dynamically scalable computing resources. Cloud computing may be supported, at least in part, by virtualization software. A cloud computing environment may be established by an enterprise and/or may be hired on an as-needed basis from a third party provider. Some cloud computing environments may comprise cloud computing resources owned and operated by the enterprise as well as cloud computing resources hired and/or leased from a third party provider.

[0052] In an embodiment, some or all of the functionality disclosed above may be provided as a computer program product. The computer program product may comprise one or more computer readable storage medium having computer usable program code embodied therein to implement the functionality disclosed above. The computer program product may comprise data structures, executable instructions, and other computer usable program code. The computer program product may be embodied in removable computer storage media and/or non-removable computer storage media. The removable computer readable storage medium may comprise, without limitation, a paper tape, a magnetic tape, magnetic disk, an optical disk, a solid state memory chip, for example analog magnetic tape, compact disk read only memory (CD-ROM) disks, floppy disks, jump drives, digital cards, multimedia cards, and others. The computer program product may be suitable for loading, by the computer system 380, at least portions of the contents of the computer program product to the secondary storage 384, to the ROM 386, to the RAM 388, and/or to other non-volatile memory and volatile memory of the computer system 380. The processor 382 may process the executable instructions and/or data structures in part by directly accessing the computer program product, for example by reading from a CD-ROM disk inserted into a disk drive peripheral of the computer system 380. Alternatively, the processor 382 may process the executable instructions and/or data structures by remotely accessing the computer program product, for example by downloading the executable instructions and/or data structures from a remote server through the network connectivity devices 392. The computer program product may comprise instructions that promote the loading and/or

copying of data, data structures, files, and/or executable instructions to the secondary storage 384, to the ROM 386, to the RAM 388, and/or to other non-volatile memory and volatile memory of the computer system 380.

[0053] In some contexts, the secondary storage 384, the ROM 386, and the RAM 388 may be referred to as a non-transitory computer readable medium or a computer readable storage media. A dynamic RAM embodiment of the RAM 388, likewise, may be referred to as a non-transitory computer readable medium in that while the dynamic RAM receives electrical power and is operated in accordance with its design, for example during a period of time during which the computer system 380 is turned on and operational, the dynamic RAM stores information that is written to it. Similarly, the processor 382 may comprise an internal RAM, an internal ROM, a cache memory, and/or other internal non-transitory storage blocks, sections, or components that may be referred to in some contexts as non-transitory computer readable media or computer readable storage media.

[0054] Having described various devices and processes herein, specific aspects can include, but are not limited to:

[0055] In a first aspect, a method of designing and testing a chemical process component, comprises: identifying the inter-relationship between different chemical process engineering parameters and structures for subcomponents of the chemical process component; defining a weighting among a plurality of dimensionless numbers associated with a processing function of the subcomponents; simulating a chemical process for each of a plurality of combinations of subcomponent designs by an application executing on a computer system to determine, for each combination, a value for each of the plurality of the dimensionless numbers; determining a simulation score by the application for each simulated chemical process based on the plurality of dimensionless numbers determined for that simulated chemical process and based on the defined weighting among the plurality of dimensionless numbers; selecting a plurality of the combinations of subcomponent designs based on the simulation scores; building a prototype of the chemical process component using a 3-dimensional printer for each of the selected combinations of subcomponent designs; testing each of the prototypes of the chemical process component; and selecting one of the prototypes based on production criteria.

[0056] A second aspect can include the method of the first aspect, wherein the production criteria comprises a product output, a waste output, or an energy consumption or a combination thereof.

[0057] A third aspect can include the method of any of the first to second aspects, wherein the plurality of combinations of subcomponent designs are selected by the application which are associated with simulation scores that exhibit mathematical inflection points or mean values between mathematical inflection points.

[0058] A fourth aspect can include the method of any of the first to third aspects, wherein the dimensionless numbers comprise at least one associated with a heat transfer chemical engineering process parameter, a mass transfer chemical engineering process parameter, a reaction kinetics chemical engineering process parameter, or a hydrodynamics chemical engineering process parameter.

[0059] A fifth aspect can include the method of any of the first to fourth aspects, wherein the dimensionless numbers comprise at least two of a Reynolds number, a Peclet number a Schmidt number, a Nusselt number, a Sherwood number, and a Graetz number.

[0060] A sixth aspect can include the method of any of the first to fifth aspects, wherein the chemical process component comprises one of a separator, a reactor, a stirrer, a mixer, or combinations thereof.

[0061] A seventh aspect can include the method of any of the first to sixth aspects, wherein the 3-dimensional printer builds the prototype using an additive manufacturing process out of one of a polymer, a plastic, a metal, or a ceramic.

[0062] In an eighth aspect, a method of building a chemical process component and using the component in a chemical processing plant, comprises: identifying the inter-relationship between different chemical process engineering parameters and structures for subcomponents of the chemical process component; defining a weighting among a plurality of dimensionless numbers associated with a processing function of the subcomponents; simulating a chemical process for each of a plurality of combinations of subcomponent designs by an application executing on a computer system to determine, for each combination, a value for each of the plurality of the dimensionless numbers; determining a simulation score by the application for each simulated chemical process based on the plurality of dimensionless numbers determined for that simulated chemical process and based on the defined weighting among the plurality of dimensionless numbers; selecting a plurality of the combinations of subcomponent designs based on

the simulation scores; building a chemical process component according to the selected combination of subcomponent designs; installing the chemical process component in a chemical processing plant; and producing a chemical product by the chemical processing plant.

[0063] A ninth aspect can include the method of the eighth aspect, further comprising building prototypes of some of the combinations of subcomponent designs selected based on the simulation scores and testing the prototypes, wherein the selected combination of subcomponent designs is selected from among the tested prototypes.

[0064] A tenth aspect can include the method of the ninth aspect, wherein the prototypes are built using additive manufacturing processes.

[0065] An eleventh aspect can include the method of any of the eighth to tenth aspects, wherein plurality of combinations that are simulated is greater than 1,000.

[0066] A twelfth aspect can include the method of any of the eighth to eleventh aspects, further comprising determining a plurality of subcomponent designs by the application, where each subcomponent design varies from other subcomponent designs by one of a change in a dimension, a quality, a geometry, or an angle.

[0067] A thirteenth aspect can include the method of the twelfth aspect, wherein the subcomponent designs vary across a predefined range of values for a dimension.

[0068] A fourteenth aspect can include the method of any of the eighth to thirteenth aspects, wherein the variation of subcomponent designs across the predefined range of values is based on performing a sensitivity analysis of variations in the design versus at least one of the dimensionless numbers by the application.

[0069] In a fifteenth aspect, a method of chemical process intensification by designing a chemical process component through modeling using dimensionless numbers, comprises: identifying the inter-relationship between different chemical process engineering parameters and structures for subcomponents of the chemical process component; defining a weighting among a plurality of dimensionless numbers associated with a processing function of the subcomponents; simulating a chemical process for each of a plurality of combinations of subcomponent designs by an application executing on a computer system to determine, for each combination, a value for each of the plurality of the dimensionless numbers; determining a simulation score for each simulated chemical process by the application based on the plurality of dimensionless numbers determined for that simulated chemical process and based on

the defined weighting among the plurality of dimensionless numbers; and selecting a combination of subcomponent designs based on each selected subcomponent design having a maximum simulation score or having a minimum simulation score.

[0070] A sixteenth aspect can include the method of the fifteenth aspect, wherein the chemical process component comprises one of a stirrer component, a mixer component, a flow enhancement component, a sampler component, a mass transfer component, a heat transfer component, a separator component, a reactor component, a distillation component, or a combination thereof.

[0071] A seventeenth the method of any of the fifteenth to sixteenth aspects, wherein the chemical process component comprises a combined separator and reactor component.

[0072] An eighteenth aspect the method of any of the fifteenth to seventeenth aspects, wherein the dimensionless numbers comprise at least two of a Reynolds number, a Peclet number a Schmidt number, a Nusselt number, a Sherwood number, and a Graetz number.

[0073] A nineteenth aspect the method of any of the fifteenth to eighteenth aspects, wherein the processing simulating the chemical process for each of the plurality of combinations of subcomponent designs comprises performing a sensitivity analysis of variations of the design versus the plurality of dimensionless numbers.

[0074] A twentieth aspect the method of any of the fifteenth to nineteenth aspects, building a plurality of prototypes using an additive manufacturing process for each of the prototypes; and testing each of the prototypes concurrently in a pilot test.

[0075] While several embodiments have been provided in the present disclosure, it should be understood that the disclosed systems and methods may be embodied in many other specific forms without departing from the spirit or scope of the present disclosure. The present examples are to be considered as illustrative and not restrictive, and the intention is not to be limited to the details given herein. For example, the various elements or components may be combined or integrated in another system or certain features may be omitted or not implemented.

[0076] Also, techniques, systems, subsystems, and methods described and illustrated in the various embodiments as discrete or separate may be combined or integrated with other systems, modules, techniques, or methods without departing from the scope of the present disclosure. Other items shown or discussed as directly coupled or communicating with each other may be indirectly coupled or communicating

through some interface, device, or intermediate component, whether electrically, mechanically, or otherwise. Other examples of changes, substitutions, and alterations are ascertainable by one skilled in the art and could be made without departing from the spirit and scope disclosed herein.

CLAIMS

What is claimed is:

1. A method of designing and testing a chemical process component, comprising:
 - identifying the inter-relationship between different chemical process engineering parameters and structures for subcomponents of the chemical process component;
 - defining a weighting among a plurality of dimensionless numbers associated with a processing function of the subcomponents;
 - simulating a chemical process for each of a plurality of combinations of subcomponent designs by an application executing on a computer system to determine, for each combination, a value for each of the plurality of the dimensionless numbers;
 - determining a simulation score by the application for each simulated chemical process based on the plurality of dimensionless numbers determined for that simulated chemical process and based on the defined weighting among the plurality of dimensionless numbers;
 - selecting a plurality of the combinations of subcomponent designs based on the simulation scores;
 - building a prototype of the chemical process component using a 3-dimensional printer for each of the selected combinations of subcomponent designs;
 - testing each of the prototypes of the chemical process component; and
 - selecting one of the prototypes based on production criteria.
2. The method of claim 1, wherein the production criteria comprises a product output, a waste output, or an energy consumption or a combination thereof.
3. The method of claim 1, wherein the plurality of combinations of subcomponent designs are selected by the application which are associated with simulation scores that exhibit mathematical inflection points or mean values between mathematical inflection points.
4. The method of claim 1, wherein the dimensionless numbers comprise at least one associated with a heat transfer chemical engineering process parameter, a mass transfer chemical engineering process parameter, a reaction kinetics chemical

engineering process parameter, or a hydrodynamics chemical engineering process parameter.

5. The method of claim 1, wherein the dimensionless numbers comprise at least two of a Reynolds number, a Peclet number, a Schmidt number, a Nusselt number, a Sherwood number, and a Graetz number.

6. The method of claim 1, wherein the chemical process component comprises one of a separator, a reactor, a stirrer, a mixer, or combinations thereof.

7. The method of claim 1, wherein the 3-dimensional printer builds the prototype using an additive manufacturing process out of one of a polymer, a plastic, a metal, or a ceramic.

8. A method of building a chemical process component and using the component in a chemical processing plant, comprising:

identifying the inter-relationship between different chemical process engineering parameters and structures for subcomponents of the chemical process component;

defining a weighting among a plurality of dimensionless numbers associated with a processing function of the subcomponents;

simulating a chemical process for each of a plurality of combinations of subcomponent designs by an application executing on a computer system to determine, for each combination, a value for each of the plurality of the dimensionless numbers;

determining a simulation score for each simulated chemical process by the application based on the plurality of dimensionless numbers determined for that simulated chemical process and based on the defined weighting among the plurality of dimensionless numbers;

selecting a combination of subcomponent designs based on simulation scores;

building a chemical process component according to the selected combination of subcomponent designs;

installing the chemical process component in a chemical processing plant; and

producing a chemical product by the chemical processing plant.

9. The method of claim 8, further comprising building prototypes of some of the combinations of subcomponent designs selected based on the simulation scores and testing the prototypes, wherein the selected combination of subcomponent designs is selected from among the tested prototypes.
10. The method of claim 9, wherein the prototypes are built using additive manufacturing processes.
11. The method of claim 8, wherein plurality of combinations that are simulated is greater than 1,000.
12. The method of claim 8, further comprising determining a plurality of subcomponent designs by the application, where each subcomponent design varies from other subcomponent designs by one of a change in a dimension, a quality, a geometry, or an angle.
13. The method of claim 12, wherein the subcomponent designs vary across a predefined range of values for a dimension.
14. The method of claim 13, wherein the variation of subcomponent designs across the predefined range of values is based on performing a sensitivity analysis of variations in the design versus at least one of the dimensionless numbers by the application.
15. A method of chemical process intensification by designing a chemical process component through modeling using dimensionless numbers, comprising:
- identifying the inter-relationship between different chemical process engineering parameters and structures for subcomponents of the chemical process component;
 - defining a weighting among a plurality of dimensionless numbers associated with a processing function of the subcomponents;
 - simulating a chemical process for each of a plurality of combinations of subcomponent designs by an application executing on a computer system to determine, for each combination, a value for each of the plurality of the dimensionless numbers;

determining a simulation score for each simulated chemical process by the application based on the plurality of dimensionless numbers determined for that simulated chemical process and based on the defined weighting among the plurality of dimensionless numbers; and
selecting a combination of subcomponent designs based on each selected subcomponent design having a maximum simulation score or having a minimum simulation score.

16. The method of claim 15, wherein the chemical process component comprises one of a stirrer component, a mixer component, a flow enhancement component, a sampler component, a mass transfer component, a heat transfer component, a separator component, a reactor component, a distillation component, or a combination thereof.

17. The method of claim 15, wherein the chemical process component comprises a combined separator and reactor component.

18. The method of claim 15, wherein the dimensionless numbers comprise at least two of a Reynolds number, a Peclet number, a Schmidt number, a Nusselt number, a Sherwood number, and a Graetz number.

19. The method of claim 15, wherein the processing simulating the chemical process for each of the plurality of combinations of subcomponent designs comprises performing a sensitivity analysis of variations of the design versus the plurality of dimensionless numbers.

20. The method of claim 15, further comprising:

building a plurality of prototypes using an additive manufacturing process for each of the prototypes; and
testing each of the prototypes concurrently in a pilot test.

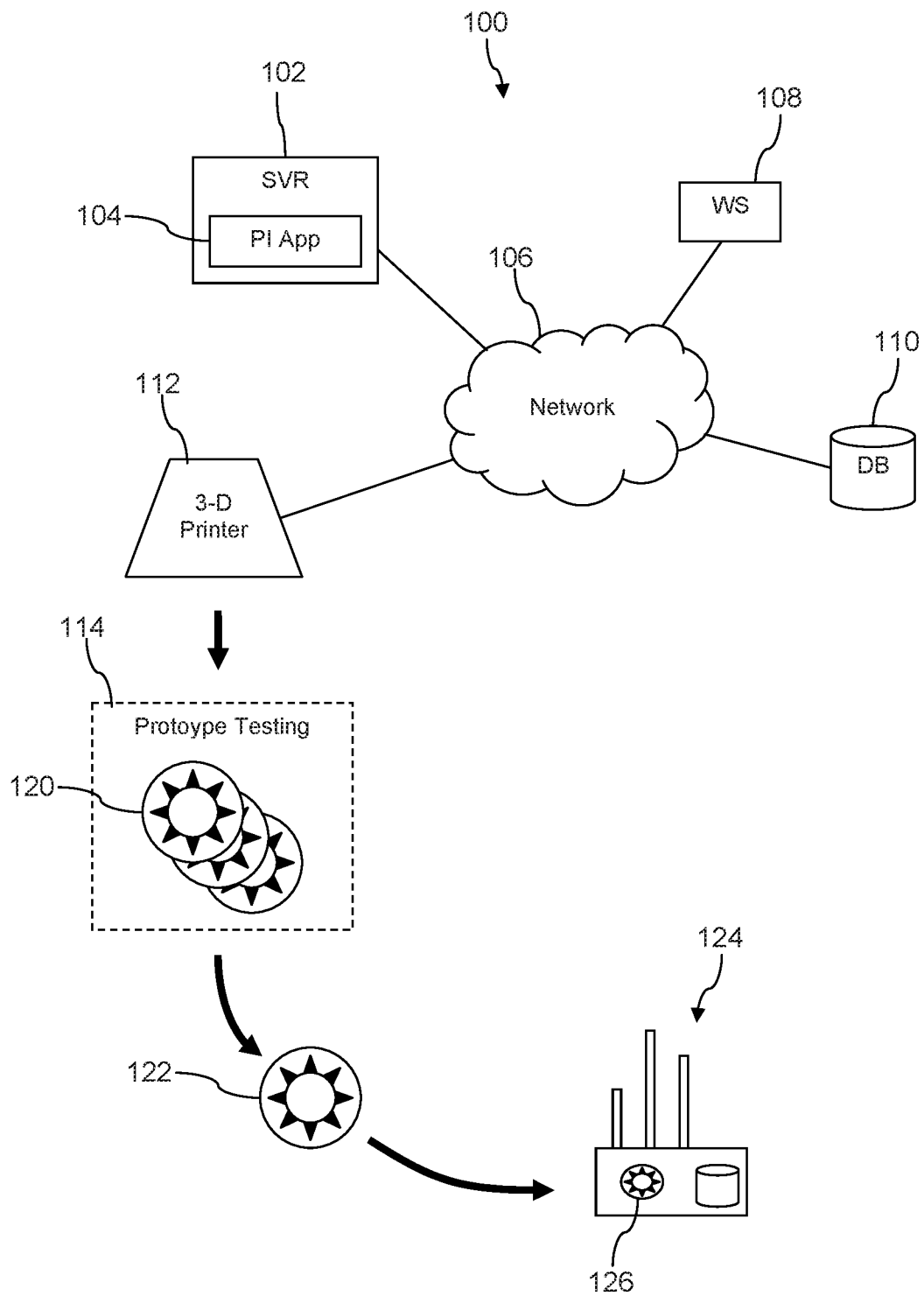


FIG. 1

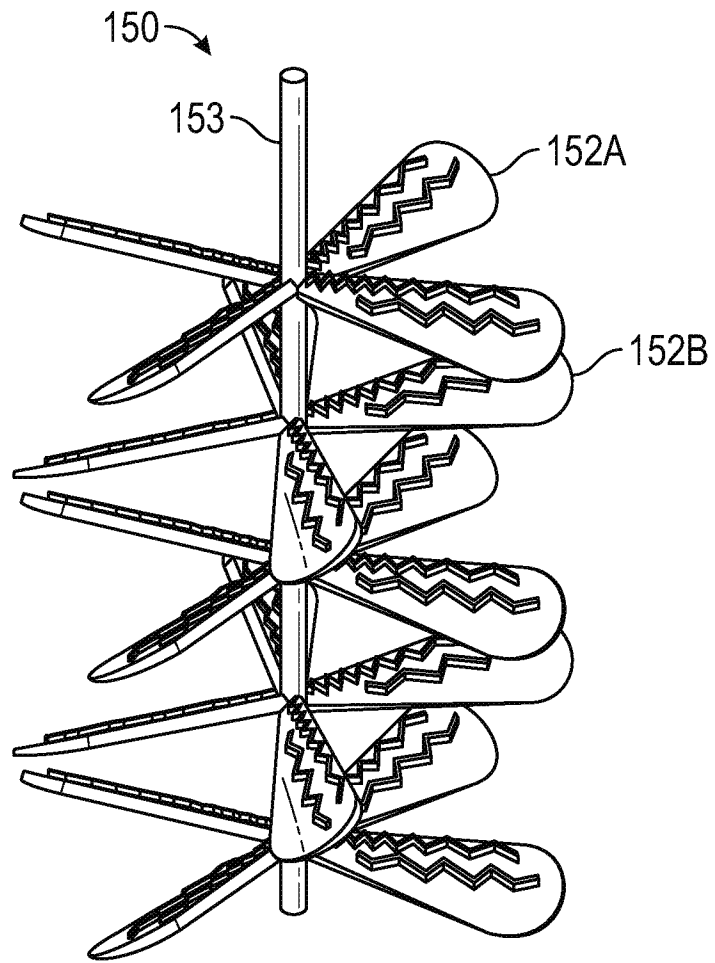


FIG. 2A

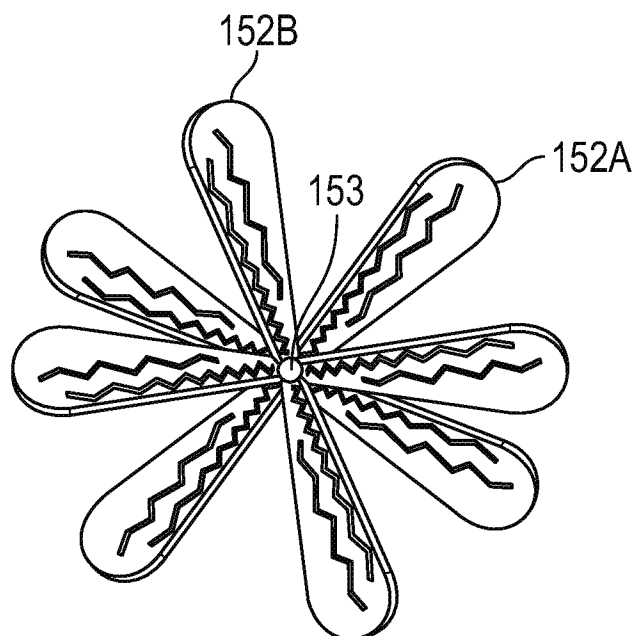


FIG. 2B

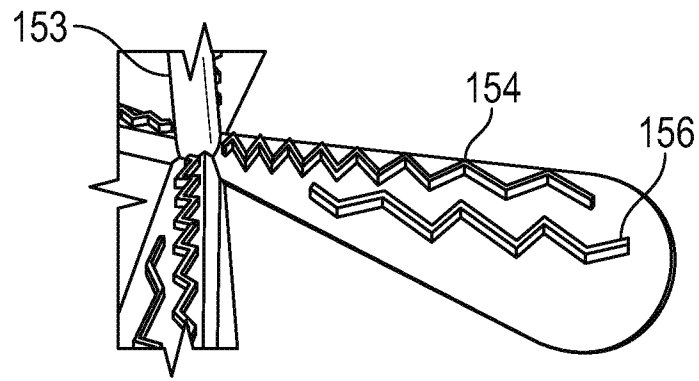


FIG. 2C

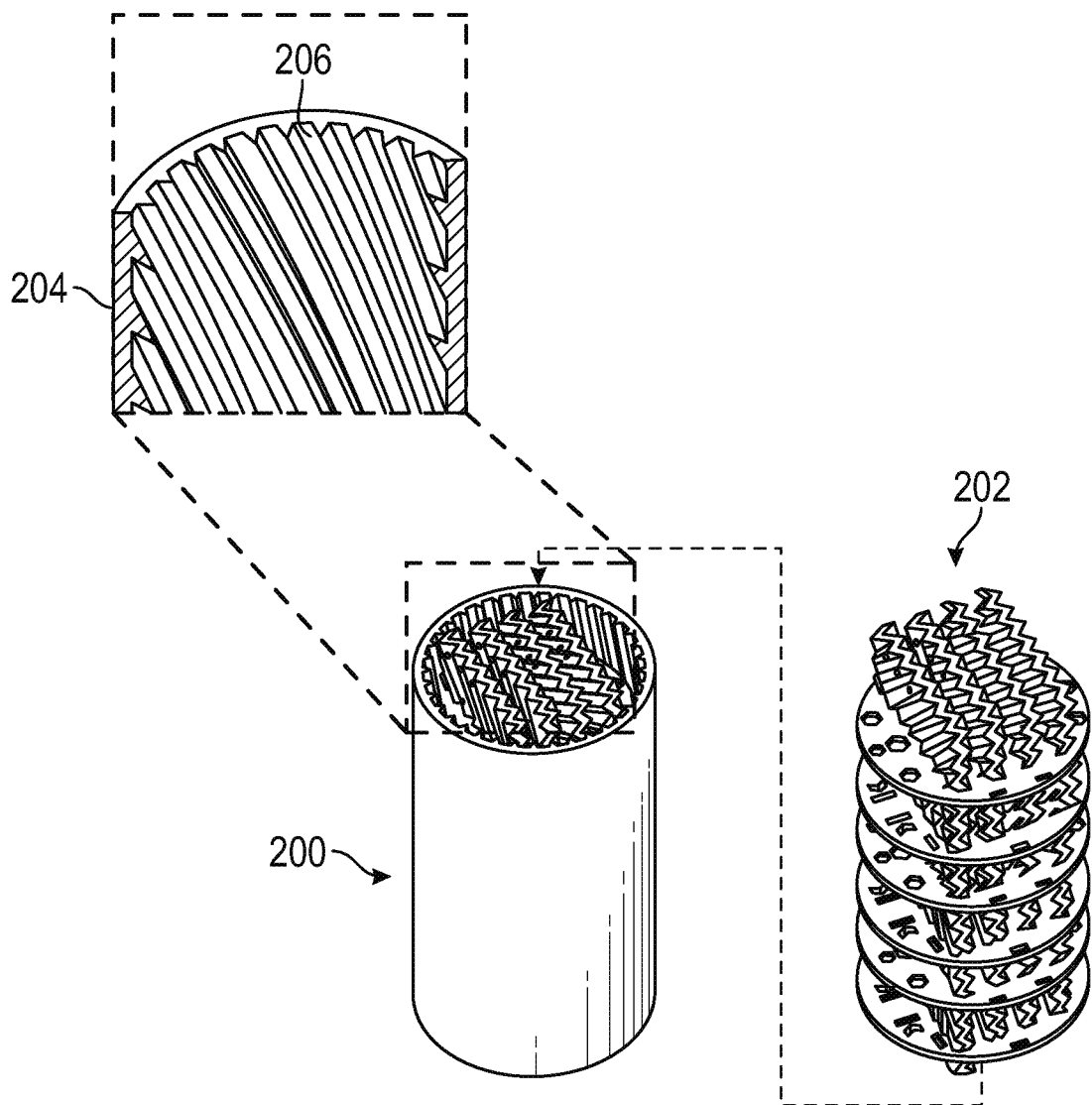


FIG. 3A

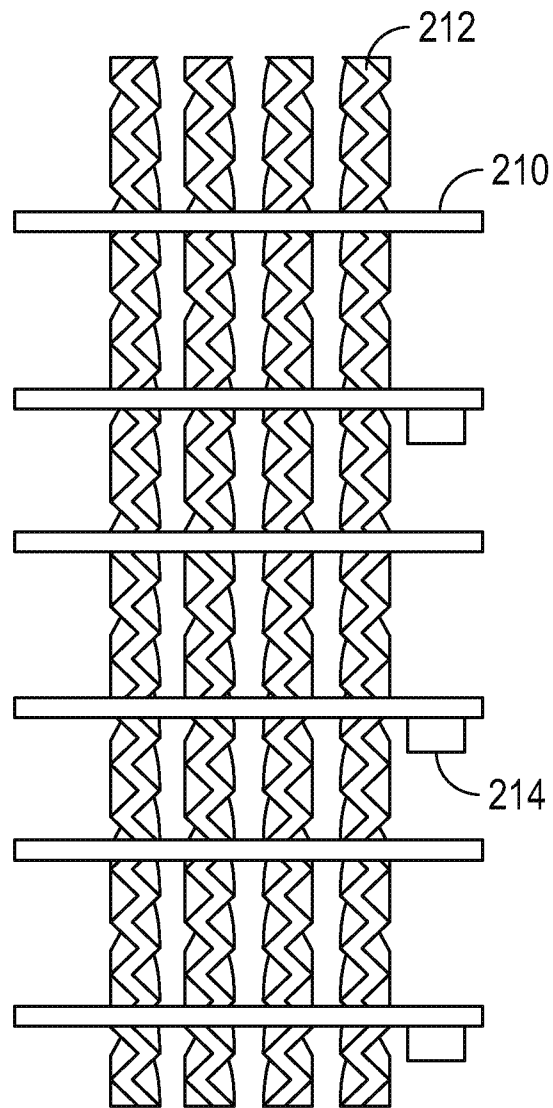


FIG. 3B

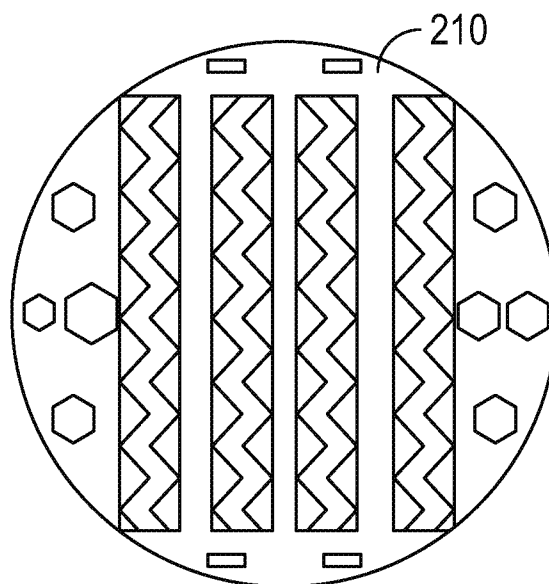


FIG. 3C

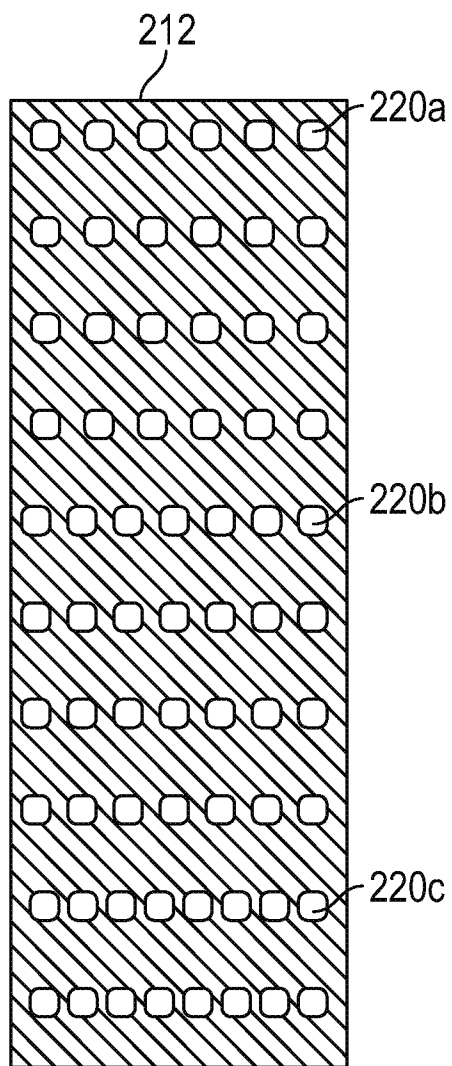


FIG. 3D

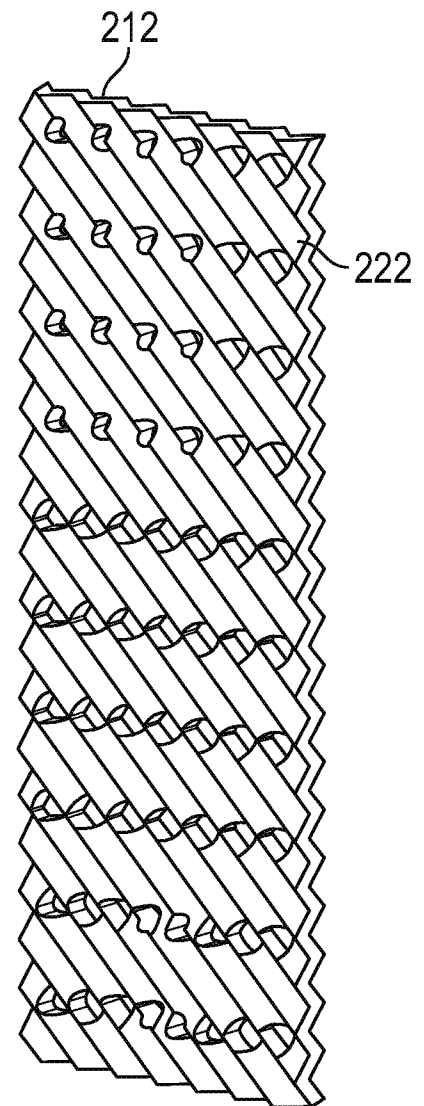


FIG. 3E

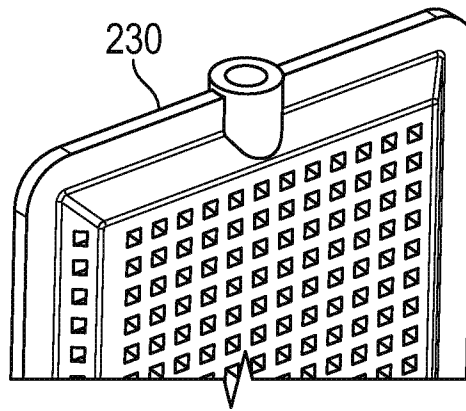


FIG. 3F

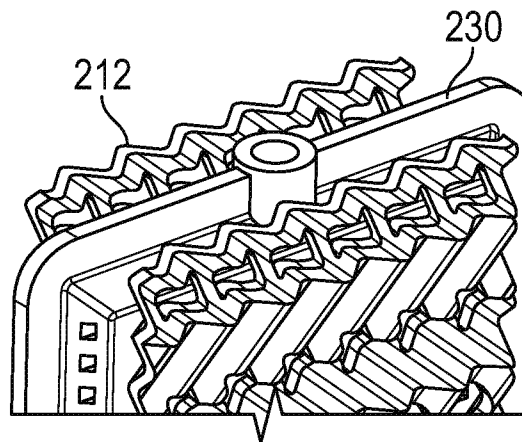


FIG. 3G

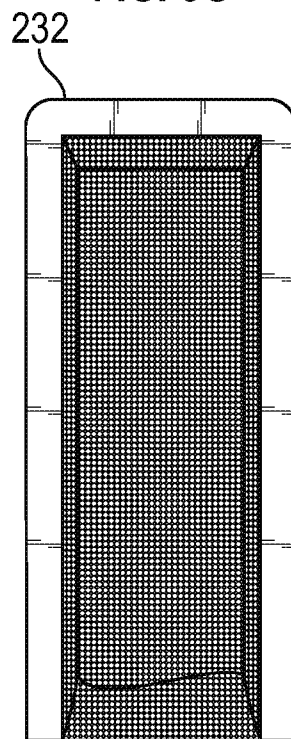


FIG. 3H

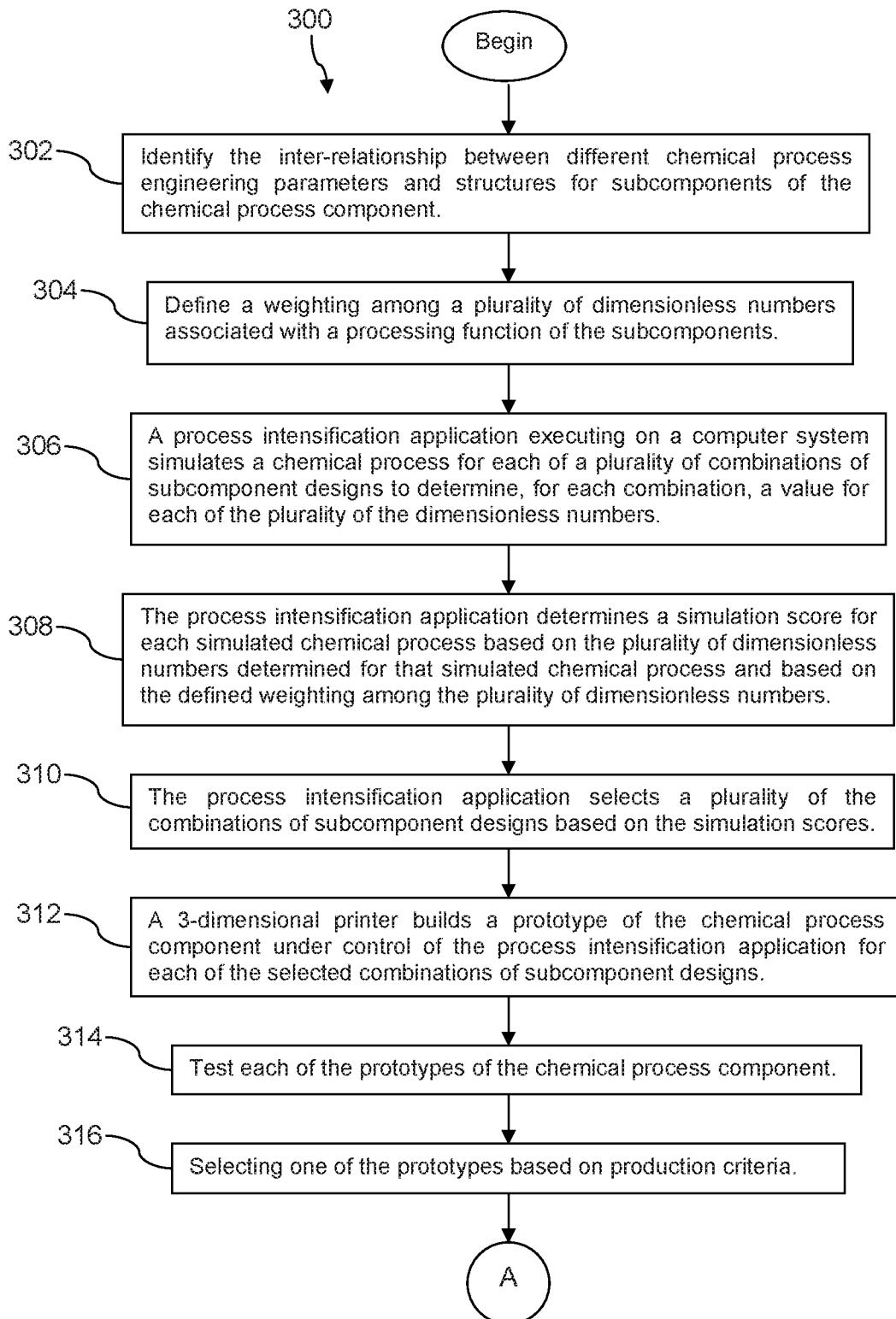


FIG. 4A

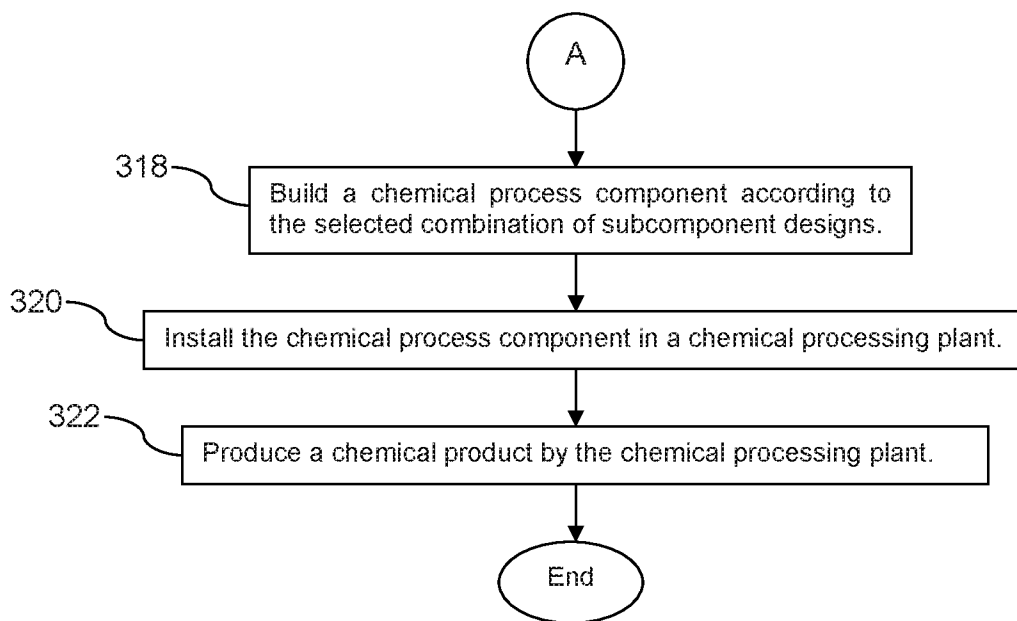


FIG. 4B

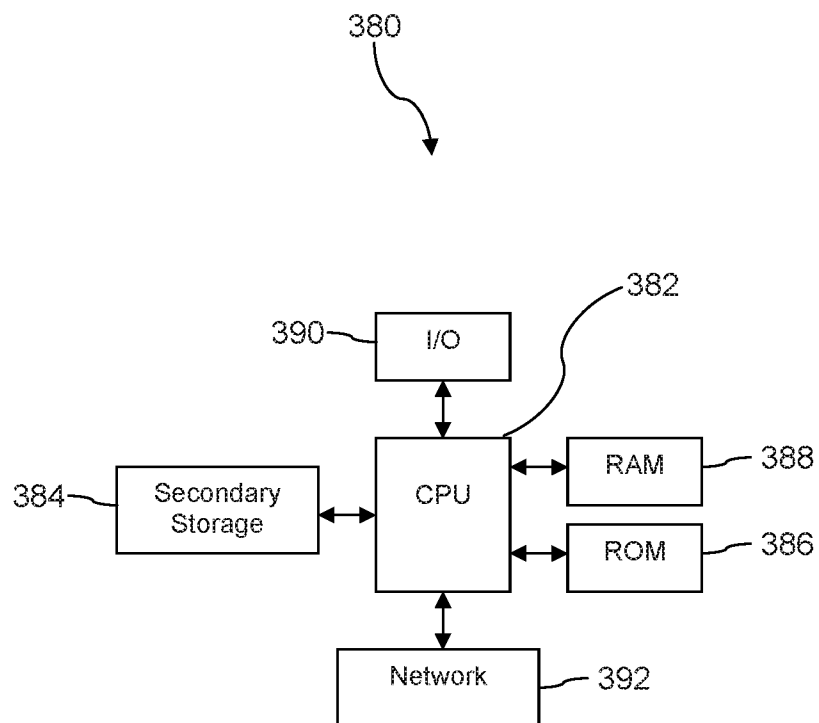


FIG. 5