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BASIC PRINCIPLES OF PROCESS MODELLING

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The principle of systems and process engineering was introduced into mathematical modelling in the middles of 20-th century by Bertalanffy, Mesarovič, Kalman, Zadeh, Benedek and others [1,2,7,9]. Himmelblau and Bischoff showed that population balance problems, i.e., processes described with another independent variable than a physical space variable, can be solved by differential equations similarly to the transport equations. Essentially the same concepts are used – even with different names – in the theory of chemical, petrochemical, ceramic, food, biochemical process engineering, building material production, metallurgy, nuclear engineering and maybe in other fields of applied chemistry or physics. The differences in the nomenclature and treatment make difficulties transferring the theoretical bases and ways of solution of different problems from one field already solved to an other one. The aim of this paper is to define the processes, so that all models shall be given a common mathematical background, all models can be deduced therefrom. The postulates listed here can also serve as definitions of processes, process engineers deal with. To sum up the main concepts of process engineering is also worthwhile to identify and support the most important I/O elements in a process approached Quality Management System for different fields of industry.

Keywords: Process modelling, principles of systems and process engineering

Introduction

In the middles of 20-th century as the principle of systems and process engineering was introduced into mathematical modelling, Bertalanffy [2] called the attention to the fact that the models describing processes functioning differently, have sometimes similar mathematical descriptions. Mesarovič [9] was the first, attending to formulate this mathematically. The mathematical system theory that could be first applied in linear cases can be regarded to Kalman [7], mostly used in control theory. The concepts of state, of the mathematical process modelling and computer simulation can also be regarded to him. Himmelblau and Bischoff [6] showed that population balance problems can be solved by differential equations similarly to the transport equations. Fan and Friedler [8], Grossman [4] and Floudas [3] have recently dealt with optimization of processes.

Essentially the same concepts are used – even with different names – in the theory of processes in different fields of applied chemistry and physics. The 1 to 3-dimensional physical spaces (length, width and depth), and other independent variables of process description, either continuous or discontinuous (like particle size, transition between phases, microorganism age, grade of polymerization, etc.) or combination thereof can be mathematically handled similarly. Even the ISO 9001:2000 standards encourage the adoption of the process approach for the management of the organisations [5]. In the standard there is explicitly written, that "any activity that receives inputs and convert them to outputs, can be considered as a process." In our paper we give some postulates which are necessarily valid for ordinary processes. We use in the following the term process for all real or theoretical systems, that satisfy the given postulates.

According to our concepts a correct process model describes process activities independently of personal wills (except environmental impacts) and do not contradict the accepted laws of classical physics. Those of relativistic and quantum physics are not taken in consideration here.

Concepts

Our aim is to present some properties of process models necessary to be *correct* in the sense that they obey the postulates below, i.e., the obvious rules of classical

Newtonian physics. The first question is whether it is a necessary condition for process models to fulfil the condition not to contradict the rules of conservation. There are two logical arguments to accept this.

First: Nobody wants to have such a process model that produces anything from nothing that is possible according to a model contradicting the rules of conservation of material. Similarly, a model contradicting the first law of thermostatics is worthless when it is applied to simulate the energy scheme of a plant. According to such a model it would be the most profitable action to produce only energy from nothing.
Secondly: Models, contradicting the rules of classical physics are valid of zero probability in practical, non-microphysical processes. It is a logically acceptable conjecture for all realistic models that parameters, estimated according to the maximum probability principle, give a better approximation of the reality also extrapolating out of their validity range.

All changes during the *process operation*[1] are due to the *state* of the process and its *environment*. The components of the state are the *conserving substances* (like mass, energy, momentum, and other conserving physical substances) that change in a process influenced only by the *environmental streams* ($s_{E,\cdot,\cdot}$). In some practical cases also other categories may be chosen as entity components, conserving their quantity during the process, changing only on environmental influences as well. Such are composition in separation or disintegration processes, the amount of chemical elements in chemical reactions, the amount of elementary nuclear particles in nuclear processes, etc.. All they are nominated as *entities*. In our formulation, we say their time–dependent distribution over the space of *process coordinates* the *process state* $\mathbf{e}_i(t)$.

The consequence of the above is that a certain process is totally specified by the initial state and by the (not necessarily time dependent) environmental streams in the time period of simulation.

The independent variables of process description are the *process variables* ($\boldsymbol{x}$) and *time* (t). Process variables span the space of process coordinates ($X \ni \boldsymbol{x}$).

The elements of the space of process coordinates are n-element variables, where n means the number of the process variables. They may be considered as *continuous* (i.e., physical space coordinates), *equidistant discrete* (i.e., grade of polymerization, serial number of units, etc.) *or abstract variables* (i.e., physical phases, crystal forms, chemical compounds, etc.). For shortness we say for them n-dimensional vectors. Time may be considered as *continuous*, *equidistant discrete*, *non–equidistant discrete* or *general time* (continuous mixed with discrete events). Continuous variables are described by continuous functions, discrete variables by sets of integer numbers, abstract variables by some single points. The set of process variables is a direct product of them, used in the process modelling.

The cardinality of the sets, both that of process variables (I) and of entity (M) is considered as finite.

Decomposition is cutting the space of process variables into two or more disjoint process variable subspaces, said *subprocesses*. Their elements are interconnected by *inner entity stream*s.

Processes are encircled by *environment*. Streams from or to it, the so-called environmental streams influence its operation. A process model including the *environmental parameters*, possibly also time-dependent, describe the dependence of their variables.

Subprocesses are linked by inner entity streams depending on the states of the connected subprocesses. They are environmental streams from the view of the subprocesses. Naturally, other variables, necessary to compute the operation or streams between the subprocesses maybe introduced within the model but not between the subprocesses, as necessary.

Subprocesses have similar properties as the processes themselves. When decomposing continuous variable processes into two or more discrete environmental variable processes at least one of them has to consist again of a continuous one.

Composition is the contrary of decomposition, i.e., building a composite model from more processes that will be subprocesses of the composed one. The process coordinates of the composed model will be the union of each subprocesses, the states are the union of subprocess states and the parameters are the union of the subprocess parameters.

Cutting a process into subprocesses has practical reason; generally only models of parts of a process can be described by an elementary or comparatively simpler model and the full process model has to be composed by them. In order to simplify the process model, usually the number of entities, process variables and parameters is reduced. This reduction results naturally in another, more inaccurate, less generally applicable model.

The operation of processes are described by *operation models* and, if they are composed of more subprocesses, by *transfer models* between them. Operation models describe the distribution of entity streams depending on the state and environmental streams. Transfer models describe the dependence of streams on the state of the connected subprocesses and some entity–independent *subprocess*. Transfers are monotonic functions of the *driving forces* i.e., of the differences/differential quotients[2] for each potential, that depends on the entity content/density of the submodel. The other factor of transfer is the *transfer coefficient* depending on the operation parameters of the submodel and on material properties, of the streams between the points connected.

The inputs of operation models are the initial state (e(0)) and their time–dependent environmental streams. The outputs of the operation model are either the actual model's state change or any functions of them.

[1] In the following: operation, where a unit operation in principle corresponds to exactly one correct mathematical operation considering the level of decomposition.

[2] We write as ·/· (e.g., content/density) if we refer to a notion, differing in our discrete/continuous treatment. The character ∅ shall not be read in the text, as in (e.g., ∅/density).

We deal only with *reproducible processes*. Reproducibility is understood that the states of processes are independent of start time: with identical state at the start time and identical environmental streams, the states of the processes are identical in any times related to the initial. This is only an abstraction; true exactly reproducible processes don't exist in the reality but can be well applied in practical modelling processes.

The second rule of thermostatics, the criterion of the increase of entropy is not dealt here with explicitly. In order to treat it, energy should divided into two kinds, regular and irregular and its motion should be constrained to one-sided. From the side of the theory, its validity is scale-dependent, what is regarded as irregular motion of particles. Also the molecular or Brownian motion of particles could be described as regular, seeing them from a molecular order of magnitude and stellar motion (movement of stellar objects) may be regarded as irregular, seeing it from a point of a higher magnitude. We omit handling these kinds of inequality constraints here. All of it is considered here is prescribing the rule that the direction of streams be always from higher potentials toward the lower. All other consequences of the second law are considered to be fulfilled by the operation models of the subprocesses.

Naturally, rules of less importance seen from the point of view of the actual problem, may be neglected in order to simplify the model. But if it has been neglected in one of the subprocesses the whole composed process model becomes more or less incorrect, concerning the left entity component

Dependent variables of a process are a finite set of entities in the case of discrete process variable functions; they are density distributions in the case of continuous process variable functions of the independent process variables. In most of the problems there are combined discrete and continuous processes.

Postulates

The first assumption put is that with correctly posed and unbounded number of measurements a process model approximates the mapping of reality. We deal only with correct models, fulfilling this assumption.

The postulates 1 to 5 are the comprised and most important component–independent features, generally accepted in the macroscopic real world.

It is claimed that

Postulate 1 *actual properties* of a process depend only on its *actual state*.

Postulate 2 *actual changes* of a process state depend only on the actual state and on the environmental streams.

Postulate 3 each process model shall obey the *conservation laws* for each *entity* component at any time.

Postulate 4 there exists at least one set of linearly independent process variables one–to–one mapping any subspace of process variable space to the space of entity content/density and to the potential functions.

Postulate 5 processes shall obey the principle of *causality*.

The next postulates express the trivial aim to the model application that results should be independent on the model users' subjective decision.

Postulate 6 If a field of process variables is built up as a union of more than one subspaces, it can be decomposed into subprocesses of the same independent variables and/or those of the same time variable.

Postulate 7 It is claimed that decomposition–composition fulfils by definition that the composition or decomposition of a process model with any initial state and environmental stream functions must result into the same environmental variable relations, independently of the mode of decomposition into any submodels.

Postulate 8 Processes are only relative–time dependent and they are independent on the zero and unit choice of time in the model.

Postulate 9 The model must be measurement–unity–invariant in time, in all its process variables and entities.

Reasons and physical background of postulates

Reason and consequence of Postulate 1: It is assumed that all material properties necessary to describe the process depend only on the actual entity content/density in the process. Simply practically there are no other impact possibilities and there is no other way of remembering on past events influencing the present or the future but the material state[3]. The fulfilment of this postulate is important in formulating models of composed processes as a complex, multivariate system of algebraic, partial difference/differential and integral equations.

Reason and consequence of Postulate 2: Streams depend on the process states and parameters – named in some cases transfer coefficients, but also rate coefficients, etc. – between the connected subprocesses. Referring to postulate 1 we obtain postulate 2. This postulate is fulfilled also for controlled processes if set points and other control variables are ordered to the process parameters.

Reason and consequence of Postulate 3: This condition is equivalent to the laws of conservation of entities, stated by definition. The sum/integral of entity changes in any process must be equal to the algebraic sum/integral of its environment streams in any time–interval/any actual time. Any sum/integral of streams must be equal zero at its junction points.

[3] This statement is difficult to see in biological processes, but sometimes it has its importance in these cases, as well [11].

Reason and consequence of Postulate 4: This postulate is a necessary condition to observe and to simulate the operation of a submodel.

Reason and consequence of Postulate 5: This postulate is trivial in everyday life. No actual or past event or observation is influenced by future environmental impacts.

Reason and consequence of Postulate 6: This postulate is valid by definition of decomposition. Contradicting this postulates the result depended on the cut, i.e., the result of simulation would depend on the subjective choice of model decomposition. Process models of the decomposed models' submodel are not necessarily of similar structure. The model state is the union of each/all its subprocess states; parameters are the union of submodel parameters. The sum/Lebesque–integral of inner streams between each/all subprocesses is zero for each entity component. Long–distance effects in process engineering are electromagnetic radiation, i.e., light and heat radiation, microwave heating, etc.[4]. These can be simulated by no–time–delay algebraic equations, while others by difference/differential equation increment models.

Reason and consequence of Postulate 8: It is a necessary condition in the everyday life. No event is influenced by the fact, whether the time is measured from the zero of the time scale, whether it is counted according to the time according to the Buddhist, Christian, Jew, Muslim, etc. calendar, or from the beginning of the operation of the invested process or from the beginning time instance of a batch process.

Reason and consequence of Postulate 9: Measurement units are on the model builder's choice, so it is impossible to influence the real operation. It is trivial that real processes are independent on the time scale shift, like in case of Postulate 8.

It should be noted that fulfilment of all the postulates is only necessary condition of practical correctness of the model. It depends also on the exactness of constitutive equations. In all of our next treatment their validity is assumed.

Process models

According to the above postulates, processes may be described by operation, composed processes by operation and transfer models between them. Operation of a composed unit would depend on the operation of all of its subprocesses. Decomposition is possible applying the philosophy of Postulate 6, in the praxis if the process can be clearly decomposed in selfstanding operation models, and in transfers connecting them.

We consider all processes possible subprocesses of a more general process, what means, it is enough to discuss process models, it includes subprocess models, as well.

In general, to simulate both the process and transfer models, the knowledge of a lot of state–property functions is needed. These functions are generally called *constitutive equations*. All of their knowledge is supposed in this treatment.

According to Postulate 1, actual properties of a process, depending on material quality, are depending only on their actual entity content/density

According to Postulate 2, actual changes of processes are depending only on the actual state of the given process, it means, on their X-space distribution.

As a corollary of Postulate 3, the sum/integral of streams or stream densities of entities is given by the sum/integral of connected streams or stream densities in any arbitrary $(\boldsymbol{x},t)$ point of the process space, regardless to the direction of the streams.

For the model of a process decomposition ***it is necessary to take in account Postulate 6***, it means the process should be decomposed into subprocesses of the same independent variables and those of the same time variable.

At last, ***the operation model has to fulfill Postulate 9***, e.g. the operation model should be dimensionally correct.

A part of the streams of the process from or to the environmental points is known, other part is unknown and we have to evaluate them. According to Postulate 6 we may assume that the equation describing the operation model fulfils the conditions for existing solution, and so it makes possible to determine the potentials of the unknown streams and the differences/derivatives of the entities with respect to the time.

The trajectories of the process – e.g. the solution of composed model – will be given by the time sum/integration of the simultaneous equation system of each operation model and of each stream model, including their initial and boundary conditions.

One of the steps is to determine all potentials depending on the density content/density of entities, that are necessary to the calculation of connected streams by the stream models. Some of the connected streams are known, others are unknown and are to be evaluated. We again assume, that the equation describing the operation model fulfils the conditions for existing solution, and so it makes possible to determine the unknown streams.

The operation model – of course – depends on the material properties, too, but they are considered as properties of the functions describing the model, so we don't discuss it in details. But we assume – according to Postulate 4 – that the functions that connect potentials and entity contents/densities are known one–to one (invertible) functions.

To simulate a process, its model has to solve the following problem:

It is necessary to determine the potentials and driving forces between the connected environmental points, based on the entity content/density of the process and its environmental points, then to determine the entity content/density corresponding to a Δt time step, using the sum/integral of the potentials and driving forces with respect to the process variables.

[4] I.e., the speed of light is considered as infinity.

By repeated application of this step, the operation model of the process can determine the entity content/density on any time–interval, also for non constant environmental streams.

Operation models

An operation model is a set of relations, describing the time dependent *state change* and the *potentials* necessary to compute the driving forces of the process toward or from its environment. The distribution of the entity content/density streams is influenced by the *constitutive relations*, by the equipment parameters of operation and by every/all streams entering and leaving the model. Operation models have to based on the constitutive equations.

Describing an operation model by its equations, in a discrete process space we have to determine the $h_j(\boldsymbol{e_i},t)$ potentials from $\boldsymbol{i}$ transfers the $\boldsymbol{j}$ subsystems and the stream rates toward or from the environment denoted by $\mathbf{v}_i(t)$. Using the notation above we get the equation for the $\Delta\mathbf{e}_i(t)$ entity change:

$$\Delta\mathbf{e}_i(t)=\left(\sum_{j\in I}\mathbf{L}_{i,j}\left(\mathrm{h}_j(\mathbf{e}_i(t))\right)+\mathbf{v}_i(t)\right)\cdot\Delta t \quad \boldsymbol{i}\in I \tag{1}$$

The first term on the right side is a sum regarding all subprocesses, defined so, that the stream is zero between subprocesses having no contact, or in the case $\boldsymbol{i}=\boldsymbol{j}$.

In continuous process space the corresponding functions are g and $\mathbf{K}_{i,j}$, similarly as the streams and the density of entities are denoted by $\mathbf{d}(\mathbf{x},t)$. The derivative of the density function with respect to the time is given by

$$\frac{\mathrm{d}\mathbf{d}(\mathbf{x},t)}{\mathrm{d}(t)}=\int_{\xi\in X}\mathbf{K}_{\mathbf{x},\xi}\left(\mathrm{g}(x,\mathbf{d}(\xi,t))\right)\mathrm{d}\xi+\mathbf{u}(\mathbf{x},t) \quad \mathbf{x}\in X \tag{2}$$

It is important to see that Postulate 3 is fulfilled if the submodels fulfil it and the composed operation models are sums/Lebesque integrals of entity on the space of process variables at any considered time. Postulate 8 and Postulate 9 are fulfilled on any time interval if the submodels fulfil them and if the composed operation models are sums/Lebesque time integrals of entity of environmental streams.

The sufficiency is clear, the necessity has not been proven according to author's knowledge, but it is of less practical importance. It is obvious in the case of transport equations.

The necessary condition of fulfilling, the laws of conservation according to Postulate 3, is given for discrete processes in Equation 3, and for continuous processes in Equation 4.

$$\Delta\mathbf{e}_i(t)=\left(\sum_{j\in I}\mathbf{r}_{i,j}(t)+\mathbf{v}_i(t)\right)\Delta t \quad \forall\boldsymbol{i}\in I \quad t\in T \tag{3}$$

$$\Delta\mathbf{d}(\boldsymbol{x},t)=\int_{t}^{t+\Delta t}\left(\int_{\xi\in X}\mathbf{q}(\boldsymbol{x},\xi,t)d\xi+\mathbf{u}(\boldsymbol{x},t)\right)dt \quad \forall\boldsymbol{x}\in X \quad t\in T \tag{4}$$

For discrete processes, the entity increase of each entity component in any process space element *i* must be the sum of all entering–leaving streams *j* connected to it; the entity increase of each entity component in any continuous process space element **x** must be the integral of entering–leaving streams on the whole process variable space and that of environmental stream connected to it.

Stream/stream density and velocity of transfers

Environmental streams in a composed model are computed by transfer models, and have to undergo the conservation rules.

Transfer between discrete submodels is interpreted as transfers of each entity belonging to them.

Transfer models of a composed process describe the dependence of transfer streams on the environmental potentials and on some entity–independent and eventually time–dependent parameters. Transfer potentials are assumed to be one–to–one functions of the entity content/density according to Postulate 2 and Postulate 4. They have to be computed either from the environment entity content/density or the potential itself by the operation models, depending eventually on the entity independent parameters of the constitutive equations. If the environmental entity capacity is considered infinite, then the potential itself has to be specified.

Transfer models are usually described as functions – mostly, but not necessarily – as products of state–dependent driving forces between the connected models and an approximately but not necessarily state–independent transfer coefficient. This is a somewhat redundant way of the stream–entity function description but is practical when the dependence is linear: the driving force equals approximately the difference of connected submodel transfer potentials, and the transfer coefficient an entity–independent constant. In this way the transfer streams depend on the driving forces that monotonously depend on the differences/derivatives of each potential and equal zero if the difference between the connected potentials is zero.

Note that such rules were motivating the first steps of physical chemistry and fluid mechanics. They are only linear approximating rules (like the Newtonian rules of heat and impulse transfer, Henry's Raoult's, rule of component transfer between fluid phases, rules of Fourier, Fick, etc.). Also such relation is for first order isothermal chemical reaction, but other reaction mechanisms are essentially non–linear.

The potentials (chemical potential, temperature, etc.) of the environment entity variables must coincide with the entity variables of the process. Environmental streams may be either time independent or dependent variables, according to the process specification.

Eq. 5 defines the velocity of entity-transfer between the points *i* and *j* in case of discrete-time processes having discrete process variables:

$$\mathbf{r}_{i,j}(t)=\left(\frac{\Delta\mathbf{e}_j(t)}{\Delta t}\right)_{i=const}=\left(\frac{\left(\mathbf{e}_j(t+\Delta t)-\mathbf{e}_j(t)\right)}{\Delta t}\right)_{i=const}\equiv$$
$$\equiv-\left(\frac{\left(\mathbf{e}_i(t+\Delta t)-\mathbf{e}_i(t)\right)}{\Delta t}\right)_{j=const}=-\left(\frac{\Delta\mathbf{e}_i(t)}{\Delta t}\right)_{j=const}=-\mathbf{r}_{j,i}(t)$$
$$\forall \boldsymbol{i},\boldsymbol{j}\in I \tag{5}$$

As one can see, the velocity in Equation 5 is defined by the partial difference quotients of $\boldsymbol{e_i}$ or $\boldsymbol{e_j}$ with respect to the time, according to this, the dimension of **r** is entity/time. This definition contains also the fulfilling of Postulate 3.

Similarly, for discrete-time processes having continuous process variables, the velocity of entity-density transfer is given in Equation 6)

$$\mathbf{q}(\boldsymbol{x},\xi,t)=\frac{\Delta(\mathbf{d}(\boldsymbol{x},t))}{\Delta t}\bigg|_{\xi\ const}\equiv-\frac{\Delta(\mathbf{d}(\xi,t))}{\Delta t}\bigg|_{x\ const}=-\mathbf{q}(\xi,\boldsymbol{x},t)$$
$$\forall \boldsymbol{x},\xi\in X \tag{6}$$

The dimension of q is entity/(generalized volume×time), the dimension of d is entity/generalized volume. In Eq. 7 and 8 is given the definition of the entity density, d , and the generalized volume, ΔV:

$$\mathbf{d}(\boldsymbol{x},t)=\lim_{\zeta\to 0}\frac{\Delta\mathbf{e}(\boldsymbol{x},t)}{\Delta V} \tag{7}$$

$$\text{where}\quad \Delta V\equiv\prod_{i\in I}\left|\Delta\boldsymbol{x}_i\right|\quad\text{and}\quad \zeta=\sup_{i\in I}\left\{\left|\Delta\mathbf{x}_i\right|\right\} \tag{8}$$

Equation 9 and Equation 10 express the velocity of entity/density -transfer for time-continuous processes having discrete/continuous process variables.

$$\mathbf{r}_{i,j}(t)=\left(\frac{\partial\,\mathbf{e}_j(t)}{\partial t}\right)_{i=const}\qquad \boldsymbol{i},\boldsymbol{j}\in I \tag{9}$$

$$\mathbf{q}(\boldsymbol{x},\xi,t)=\left(\frac{\partial\,\mathbf{d}(\boldsymbol{x},\xi,t)}{\partial t}\right)_{\xi=const}\qquad \boldsymbol{x},\xi\in X \tag{10}$$

Phenomenological description of stream/stream density

The $\mathbf{q}(\mathbf{x},\xi,t)$ entity density-transfer stream velocity between points **x** and ξ is defined usually as the product of an entity-transfer coefficient and of the driving force. The entity-transfer coefficient is usually – but not in all cases – described by the $\mathbf{L}_{i,j}(\mathrm{h}_j(\mathbf{e}_i(t))$ transfer coefficient, depending on the entity content of the subprocesses and on the geometry describing their contacts (for example heat transfer coefficient in discrete state space or heat conduction coefficient in continuous state space.), and by the potential difference vectors – called the driving force vectors – as their component–by component product.

The above mentioned decomposition is not a unique one, but it is very useful for linearization, because the entity-transfer coefficient may be regarded often constant, and the driving force can be considered as proportional with the entity-differences, which means a considerable simplification in the numerical steps of the simulation.

Considering the above mentioned, the transferred entity stream/density between any arbitrary two discrete time points from $\boldsymbol{x}_2$ toward any $\boldsymbol{x}_1$ points is given by

$$\Delta\mathbf{e}_i(t)=\sum_{\forall j\in I}\mathbf{r}_{i,j}(t)\cdot\Delta t=\left(\sum_{\forall j\in I}\left(\mathbf{L}_{i,j}\left(\mathrm{h}_i\left(\mathbf{e}_j,t\right)\right)-\mathbf{L}_{j,i}\left(\mathrm{h}_j\left(\mathbf{e}_i,t\right)\right)\right)\right)\cdot\Delta t\quad\forall i\in I \tag{11}$$

The number of equations describing these conditions is $\mathrm{n}(I)^2$. In the case of $\boldsymbol{i}=\boldsymbol{j}$ Equation 11 is an identity, thus is meaningless.

Similarly, Equation 12 describes the entity-change rate in case of continuous process variables:

$$\Delta\mathbf{d}(\boldsymbol{x},t)=\int_{\xi\in\Delta V}\mathbf{q}(\boldsymbol{x},\boldsymbol{\xi},t)\,\mathrm{d}\boldsymbol{\xi}\cdot\Delta t=$$
$$=\int_{\xi\in\Delta V}\left(\mathbf{K}_{\boldsymbol{x},\xi}\left(g(\mathbf{d}(\boldsymbol{x},\boldsymbol{\xi},t))\right)-\mathbf{K}_{\xi,\boldsymbol{x}}\left(g(\mathbf{d}(\xi,\boldsymbol{x},t))\right)\right)\mathrm{d}\boldsymbol{\xi}\cdot\Delta t \tag{12}$$

The functions **K** and **L** are nonnegative, and invariant to interchanging of the points $_1$ and $_2$, necessarily for all entity components of any subsystems.

Streams can belong to more than two contact points, as well. (Like in chemical reactions between more than two molecules).

Primary model

Here we don't deal with functions describing operation of elementary models. We assume, those are well known either from the theoretical background of the process or from some empirical equations.
But fulfilling the postulates discussed above, is required for the primary models, as well.

Composed model

The solution of a composed model means that we know all the trajectories of the subprocesses, i.e. the entity contents and all the streams at all possible time point is determined.

In case of a composed model the solution is given by the simultaneous solution of a multidimensional, usually non–linear, perhaps in closed form not known, partial integro–differential equation (including initial and boundary values). This integro–differential equation is given by all of the operation models and by all of the stream models. The simultaneous solution of this p.d.e. gives the derivative of the processes, from that the trajectories can be determined. Usually we don't have general solution in closed form, but only numerical ones by Euler, Newton, Broyden, etc. methods.

Some usual notions

Velocity: Entity/density velocity is an often-occurring concept in process engineering. It is difficult to define in the process variable spatial description but may be defined as the absolute value of the difference–quotient/gradient of the mass components of entity on the process subspace: length, width and deepness. The gradient direction of energy–stream and velocity are often but not necessarily taken as equal to the former. Generally speaking, each entity component has its own velocity.

Conductive streams: Conductive streams (like molecular diffusion, heat conductivity, etc.) are often occurring in the so–called transport equations as second order difference/differential terms. The description of such conductive streams is possible, taking into consideration the entity contents/densities in all points of the considered space with proper weights. In the practice they can be simplified into the usual second order differential equations (divergence or rotation). This way of describing conductive streams is strongly exhausted in the so called transport equation in the theory of chemical process engineering. In our further treatment it will be not discussed; it is left for the future.

Cross effects: In most of the cases the so–called cross effects can be neglected between the component entity Ø/density and the energy or impulse transfer streams[5]. In some cases they are also applied in industrial processes, like thermodiffusion in isotope separation. If necessary, they can be taken into consideration using vector–vector equations instead of particular relations to compute each transfer coefficient.

Pressure, pressure drop: The theoretical base of pressure and pressure drop computation is the law of conservation of momentum, transferring the momentum change by the pressure drop to the ground. Its value is computed from the state, its change by the Navier–Stokes equation. In most of the cases, however, the change calculation is simplified calculating the pressure drop by friction factors.

Linear models in the space of process coordinates

Linearity in the space of process coordinates

A process model is said to be *linear in the space of process coordinates* (further l.p.c.) if the

Equation 13

$$\mathbf{e}\left(c_1 \cdot z_1 + c_2 \cdot z_2\right) = c_1 \cdot \mathbf{e}\left(z_1\right) + c_2 \cdot \mathbf{e}\left(z_2\right)$$

holds for any two $z \in X \cup U$ points of the union of the space of process and environment variables. According to this definition is easy to see that if an operator l.p.c. contains parameters, they have to be independent of z.

If such a model is a linear approximation of a continuous and differentiable non–linear model its coefficients become the corresponding partial difference/differential quotients of the variables on the corresponding (discrete or continuous) time variable. The simulation result becomes

the sum of the state changes in time differences in discrete processes, and

the time integral of the state changes in time in continuous time processes.

It is easy so see that time independent processes have to be time independent as well. In all cases the models can be discrete or continuous in time. Nothing is against that subprocesses of a l.p.c. process be nonlinear, supposed that their corresponding partial difference/differential quotients are approximated by state independent values.

The coefficients of the linear system are given by the Equation 11 and Equation 14:

$$\mathbf{0} = \mathbf{L}_{i,j}\left(\mathbf{e}_j, \mathbf{e}_i, t\right) \cdot \mathrm{h}\left(\mathbf{e}_j(t)\right) - \mathbf{L}_{i,j}\left(\mathbf{e}_j, \mathbf{e}_i, t\right) \cdot \mathrm{h}\left(\mathbf{e}_i(t)\right) \quad \forall i, j \in I \tag{14}$$

$$\mathbf{0} = \mathbf{K}_{x,\xi}\left(\mathbf{d}_\xi, \mathbf{d}_x, t\right) \cdot \mathrm{g}\left(\mathbf{d}_\xi, t\right) - \mathbf{K}_{\xi,x}\left(\mathbf{d}_\xi, \mathbf{d}_x, t\right) \cdot \mathrm{g}\left(\mathbf{d}_x, t\right) \quad \forall \boldsymbol{x}, \boldsymbol{\xi} \in X \tag{15}$$

If the problem is linearized, all coefficients $\mathbf{L}_{i,j} \cdot \mathrm{h}(\mathbf{e}_j)$ of Equation 11 and Equation 14 are constants. It can be described clearly by hypermatrix – hypervector notation. For lack of space, it is omitting here.

One of the most problematic cases is dividing homogeneous streams, that needs a prescription of entity stream ratios. It has to be described by bilinear equations that restricts the validity of the linearized equations into small time steps. That's why networking programs have to iterate the concentration at each stream recirculation, too.

An algorithm for the solution

Considering the above mentioned model descriptions, we suggest the following algorithm for the solutions:

1. Having determined the derivatives of each entity content and each entity stream functions for each subprocess, we have to solve the corresponding system of linear equations. These procedures result an approximating linear system, whose accuracy depends on the length of the applied steps. This linear system won't be more complicated if we consider as variables not only the entity contents of the subprocesses, but those of the higher level processes, too.
2. The next procedure is to evaluate the roots of the approximating linear system, that makes possible to approximate the next time-step values of the streams using Euler, Newton, Broyden, or other methods
3. We add the resulted entity changes to the corresponding previous entity values.

4. We do this procedure until the last time point will be reached.

Theoretically the method offers the possibility for the numerical approximation of the trajectories also in the case of non–constant environmental streams. Of course, the numerical differentiation in each step could require a long computer time if the number of subprocesses is high.

The goal of the most computer engineering problems is to determine the stationary state of a stable system. This goal, considering constant values of the environmental variables (theoretically) can be reached if we know the coefficient matrix of the linear model: it requires the numerical solution of the eigenvalue–eigenvector system corresponding to the coefficient matrix of the dynamic simulations equation system.

We don't suggest any method to determine the process variables or to carry out the decomposition. Both problems need special engineering aspects for each individual problem. The regularity of the corresponding Jacobian matrix offers only a checking possibility. Decomposition usually expands the number of parameters, but in case of linear models the huge equation system splits into several smaller ones, so that it offers bigger accuracy of numerical approximation. Inversely, if we patch up subprocesses, the number of parameters decreases. Sometimes it is necessary to shorten the intolerable long computing time, satisfied with lower accuracy of numerical approximations.

These models are important, showing the theoretical possibility of simulation and optimizing complex processes, built up from subprocess models. We can also see the problem inversely: how a process may be seen from above, yielding a product wanted, decomposing it into subprocesses such detailed as it is necessary to reach the accuracy wanted. We are continuously working on some examples describing very different fields of process engineering, which show well the common bases and sometimes different ways of solving the complex process simulation and optimization problems.

Conclusions

However, processes have been designed and industrially applied for centuries, the theory of their simulation, based on correctly formulated and defined basis, has not clearly put yet, according to the authors knowledge. The postulates put in this paper show some theoretical bases of simulation and process design and inspire a theoretically exactly based way of computing. The reason, not to formulate these rules is possibly due to the difficulty of executing such a calculation. This seemed to be impossible by human forces and to computers too up to the last decades. However, the computation possibilities reached in last years such a speed and memory capacity that the computation, necessary to such a simulation is over or shall reach them in few years. This paper tries to give basic postulates, some of them based on the well–known rules of physics and others on trivial logical statements. Naturally, the question on the knowledge of constitutional equations remains.

Applying the algorithm outlined would be able to simulate, design, optimize processes, design their control system, their sensitivity on input, their stability.

The stochastic simulation has not been treated here, in that case the objects are not numeric but probability distributions and the theoretical treatment becomes more complicated. One must not forget applying also the deterministic simulation model the chaotic uncertainty of the result due to the inherent sensitivity on initial conditions of such systems.

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List of Symbols

cont. pr.	continuous process
disc. pr.	discrete process
$\mathbf{d}(\mathbf{x},t)$.	density of an entity
$e_i(t)$	time dependent distribution of an entity
$g(\mathbf{d}(\mathbf{x},t))$	potential in a cont. pr.
$h(\mathbf{e}_i(t))$	potential in a discrete process
$\boldsymbol{i}$ or $\boldsymbol{j}$	a discrete process variable vectors
I	the set of disc. proc. variable vectors
M	the set of entities
$\mathbf{L}_{i,j}$	entity transfer coefficient for disc. proc. variables
$\mathbf{K}_{x,\xi}$	entity transfer coefficient for cont. proc. variables
$\mathbf{r}_{i,j}(t)$	velocity of entity transfer
$\mathbf{q}(\boldsymbol{x},\boldsymbol{\xi},t)$	velocity of entity density transfer
s, σ	streams
t	time
T	the set of time values
$\mathbf{v}_i(t)$	environmental stream vector (discr. pr.)
$\mathbf{u}(\boldsymbol{x},t)$	environmental stream vector (cont. pr.)
$\boldsymbol{x}$ or ξ	process coordinate vectors
$\boldsymbol{X}$	the set of cont. proc. variable vectors
ΔV	generalized volume
ζ	factor for the definition of $\mathbf{d}(\mathbf{x},t)$.

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