



SHORT AND LONG TIMESCALES IN RECYCLES

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Abstract

A new awareness on modelling is growing in the control-oriented community recognising the fact that control is dominantly model based. Since control is about manipulating certain characteristics of the plant, it is no surprise that modelling for control focuses on extracting exactly those characteristics of the plant that are to be controlled. This invariably induces the use of time scale assumptions and consequently model reduction methods. These assumptions lead to a time-scale separation, which results in a layered control structure, with the control loops getting slower as one moves upwards in the hierarchy of time-scales.

Recycle structures are very common. The components may be fast, but the overall structure including the loop is usually much slower because of the recycle. These structures thus lend themselves to the application of time-scale assumptions. We demonstrate that any of these structures can be analysed. Starting with a first-principle based representation that makes no particular assumption on the nature of the process except that of a large recycle and fast internal dynamics, we derive a first-order approximation of a system. The result is generic and not dependent on the particular nature of the individual processes other structural properties of the process.

Keywords: Computer-aided, modelling, model reduction, process systems engineering, control

Background

One observes that currently larger and larger systems are being controlled and since the control methods are increasingly model based, the dimensionality of the model becomes a serious issue [2]. In many cases, whilst the control algorithms are available, computing is not up to solve the thus-formulated problems in real-time. It is also observed that one often gets quite satisfactory results from low-order models, which brings about the thought that one should be able to extract the control-relevant dynamics from the complex models and use the reduced-order model instead for control [1]. Feedback makes control rather robust to a certain class of modelling errors. Order of the approximation is one of them, if one does not insist on very fast control. The consequence of this thinking leads in recent years to a revitalisation of model reduction based on time-scale assumptions.

Time-scale assumptions are done all the time when modelling processes. Mostly assumptions seem to just "occur" – they are mostly done intrinsically, for example one makes the assumption of an ideally-stirred tank reactor, which in terms of time scales implies that the internal flows are much faster than the flows in and out of the tank. For the illustrative example, we shall use an abstraction introduced by this group over the past years as part of the Modeller project [4, 5, 7] to demonstrate that any recycle process can be captured in this framework. Thus models, such as they are published in for example [3], which also motivated this derivation, fold into the discussion below and in terms of assuming event dynamics for reactions into [4] thus covering the two important domains of time scale assumptions made in process engineering.

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Proposition

Processes with (multiple) internal recycles exhibit in the large time scale uniform intensities in the recycle and in the fast time scale, a change in the input will result in an internal profile of the intensities. The time scales introduced are related to the dynamics of the capacitive elements in the recycles¹.

More precisely, in the **large time scale**, slow changes in the continuous (positive) input will result in a uniform profile of the intensive quantities if the internal time constants are relatively small. Also, pulses of extensive quantity spread instantaneously in the recycle's capacitive elements. On the **short time scale** the effects invert: the slow variations in the positive input streams have no visible effect on the intensities of the elements in the recycles and fast injections cause a distribution in the intensities.

Process Definition

For the analysis we choose a general recycle process, which consists of a number of capacitive elements² in the recycles and in general any number of inflows and outflows. For the purpose of simplicity but without any limitation to the applicability of the result, though, we limit the process to one inflow and one outflow. Furthermore, we firstly limit the discussion to a single recycle process, which readily extends to a multiple, interlocking recycle process later. The choice of the model is motivated by such models as they were used in [6] but also models that are constructed in computational fluid mechanic packages. We assume that no transformation of extensive quantity (i.e. mass transformation in the form of reaction) or a very fast transformation is taking place in the plant. In the figures, the circles represent capacitive elements, here modelled as single lumped systems. The arrows mark mass flow, here for simplicity unidirectional, that is, the flow does not change direction during the viewed time period. The plant has two special elements, namely the one where the input stream enters the recycles, here labelled with 1 and the one where the outflow is attached, here shown as e . The generic element in

¹It will be necessary to make assumptions about the distribution of the relative dynamics of the elements in the recycles asking for relative uniform distribution.

²What is here called *capacitive element* is in other parts of the literature often called *compartment*

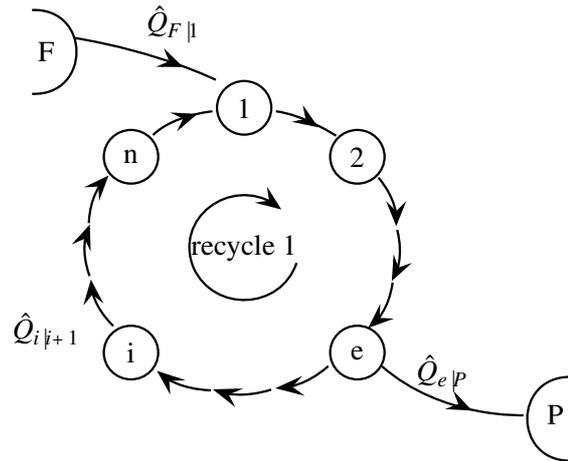


Figure 1: A one recycle, one-input, one-output process. The recycle represents the plant being modelled. The plants environment has two elements both reservoirs, that is infinitely large capacities. The F indicates the feed reservoir, the P the product reservoir. The lump i is an arbitrary system in the recycle without an inflow or an outflow to the environment. The system 1 is where the inflow is connected and the outflow is connected at the element e .

the cycle is labelled with an i .

The basic dynamic equations are then the conservation of fundamental extensive quantities, Q for each lump, which balance the change in the system with the in and outflows of fundamental extensive quantity, \hat{Q} :

$$\begin{aligned} \frac{dQ_1}{dt} &= \hat{Q}_{n|1} - \hat{Q}_{1|2} + \hat{Q}_{F|1}, \\ \frac{dQ_e}{dt} &= \hat{Q}_{e-1|e} - \hat{Q}_{e|e+1} - \hat{Q}_{e|P}, \\ \frac{dQ_i}{dt} &= \hat{Q}_{i-1|i} - \hat{Q}_{i|i+1}. \end{aligned}$$

With the appropriate definitions these equations are cast into a matrix equation:

$$\frac{d\mathbf{Q}_I}{dt} = \underline{\mathbf{A}}_1 \hat{\mathbf{Q}}_I + \underline{\mathbf{B}}_E \hat{\mathbf{Q}}_E. \quad (1)$$

In what follows, we shall refer to the matrix $\underline{\mathbf{A}}_1$ as the *recycle matrix*, here the one stands for recycle one. The two matrices $\underline{\mathbf{A}}_1$ and $\underline{\mathbf{B}}_E$ are direction coefficient matrixes for the internal flows and the external flows, respectively and represent the graph of vertices (capacities) and arcs (flows):

$$\begin{aligned} \underline{\mathbf{A}}_1 &:= \begin{pmatrix} -\underline{s}_1 + \underline{s}_2, & -\underline{s}_2 + \underline{s}_3, & \dots, & -\underline{s}_n + \underline{s}_1 \end{pmatrix}, \\ \underline{\mathbf{B}}_E &:= \begin{pmatrix} \underline{s}_1, & \underline{s}_e \end{pmatrix}. \end{aligned}$$

\mathbf{s}_i :: vector with zeros with a 1 at the i^{th} position.

The basic model balances an arbitrary fundamental extensive quantity, which we denoted with Q . The Q is thus placed into the role of the state. The proposition suggests that we expect the intensities in the recycle to converge to the same level. This makes it necessary to introduce a state variable transformation changing the representation from the fundamental extensive quantity, being the state, to an arbitrary intensive variable being the state. For this purpose, we have to introduce a second extensive quantity q , which is used to norm the fundamental extensive quantity Q , thereby defining the arbitrary intensive quantity: $\xi := \frac{Q}{q}$. The second extensive quantity is usually chosen such that it changes only insignificantly as a consequence of the process. Often it is a quantity such as volume, which implies assumptions on the changes of the volume with flow conditions and concentration changes. These are order-of-magnitude assumption. If indeed a second fundamental extensive quantity is chosen, we need to label the fundamental extensive quantities: $\xi := \frac{Q^a}{Q^b}$. Both will satisfy the balance equations (1). Rewriting the balance equations for the fundamental extensive quantity Q^a one finds:

$$\frac{d\mathbf{Q}^b \xi_I}{dt} = \underline{\mathbf{A}}_I \hat{\mathbf{Q}}_I^b \xi_I + \underline{\mathbf{B}}_P \hat{Q}_{e|P}^b \xi_I + \mathbf{b}_F Q_{F|I}^b \xi_F,$$

with the matrices $\underline{\mathbf{Q}}^b$ and $\hat{\mathbf{Q}}_I^b$ being diagonal matrices. The index I is used to mark internal quantities, such as internal flows. The recycle matrix $\underline{\mathbf{A}}_I$ is not changed, whilst the factor with the direction matrix $\underline{\mathbf{B}}_E$ is split into two. The second part describes the inflow part (term with \mathbf{b}_F) and the first part describes the outflow part (term with $\underline{\mathbf{B}}_P$). This bi-sectioning is a reflection of the fact that the streams inherit the property of the source system. Since we assumed unidirectional flow, the inflow inherits the properties of the feed system and the outflow the one of the system where it is connected to the recycle, namely the system labelled e. The outflow part, is the vector \mathbf{s}_e padded with the appropriately sized zero matrix to form the $\underline{\mathbf{B}}_P$ matrix such that this matrix operates on the full internal intensive property vector ξ_I .

This representation is readily extended to multiple-recycle systems. For each recycle a term with a recycle matrix is added. Because the dimension of the model changes, the other matrices are

padded with zero blocks accordingly.

$$\frac{d\mathbf{Q}^b \xi_I}{dt} = \left(\sum_r \underline{\mathbf{A}}_r \hat{\mathbf{Q}}_I^b + \underline{\mathbf{B}}_P \hat{Q}_{e|P}^b \right) \xi_I + \mathbf{b}_F Q_{F|I}^b \xi_F \quad (2)$$

The vector ξ_I is a collection of the intensities of all plant-internal subsystems. The running index r indicates the recycle loops. The further extension to the case of multiple inflows and outflows are also readily accommodated by modifying the $\underline{\mathbf{B}}_P$ -matrix and \mathbf{b}_F -vector as well as the inflow intensity vector accordingly.

Time Scale Analysis

In the large time scale two extreme cases are of interest. Firstly, it is of interest to analyse the behaviour of the fast part of the plant, here the internal recycles, as the external flows are changing on the large time scale, namely slowly. Secondly it is the response to very fast changes, approximated by impulses, of the fast part of the plant, though on the large time scale.

Slowly Changing Inputs (Approx. Const.)

For the **first case**, the internal system will approach the equilibrium when making the order-of-magnitude dynamics assumption of a constant input. Thus for the fundamental extensive quantity Q^a we can write using the intensities:

$$\mathbf{0} = \underline{\mathbf{A}}_I \hat{\mathbf{Q}}_I^b \xi_I + \underline{\mathbf{B}}_P \hat{Q}_{e|P}^b \xi_I + \mathbf{b}_F \hat{Q}_{F|I}^b \xi_F, \quad (3)$$

which has the solution: $\xi_I = \mathbf{e} \cdot \xi_F$

Proof. The latter is proven easily by noticing the fact that both fundamental extensive quantities satisfy the balance equation. Thus

$$\mathbf{0} = \underline{\mathbf{A}}_I \hat{\mathbf{Q}}_I^b + \mathbf{s}_e \hat{Q}_{e|P}^b + \mathbf{b}_F \hat{Q}_{F|I}^b,$$

and by rewriting the vector of extensive quantities as the product of a diagonal matrix, the said vector as diagonal, with a vector of ones $\mathbf{e} := [1, 1, \dots, 1]^T$, and noticing that $\mathbf{s}_e := \underline{\mathbf{B}}_P \mathbf{e}$, the desired form is obtained:

$$\mathbf{0} = \underline{\mathbf{A}}_I \hat{\mathbf{Q}}_I^b \mathbf{e} + \underline{\mathbf{B}}_P \hat{Q}_{e|P}^b \mathbf{e} + \mathbf{b}_F \hat{Q}_{F|I}^b \mathbf{e}.$$

It is now apparent that

$$\underline{\mathbf{b}}_F \hat{Q}_{F|}^b := - \left(\underline{\mathbf{A}}_I \hat{Q}_I^b + \underline{\mathbf{B}}_P \hat{Q}_{e|P}^b \right) \mathbf{e},$$

which when substituted into equation (3) yields

$$\underline{\mathbf{0}} = \left(\underline{\mathbf{A}}_I \hat{Q}_I^b + \underline{\mathbf{B}}_P \hat{Q}_{e|P}^b \right) \left(\underline{\xi}_I - \mathbf{e} \xi_F \right)$$

proving the fact of the solution to equation (3). \square

Keys

Assumption *The dynamics of the input is assumed slow, so slow that it does not change significantly in the time scale of the fast process.*

Assumption *Internal process dynamics are fast compared to external dynamics.*

Result *Intensities approaches equilibrium quickly.*

Result *Internal intensities are uniform and identical to the input, in the single input case, otherwise the weighted average.*

Result *At steady state, all extensive quantities do not change, thus norming may be done with any extensive quantity.*

The last statement is worth elaborating: Often the volume is chosen as the norming extensive quantity. As the above analysis shows, the requirement of being conserved is implied. If the result is applied to slowly changing inputs, the volume, the density and the internal volumes are not to change significantly.

A Slightly More Restricted Model

For the further development, we first generalize our model and use the above-given definition for the intensity. The norming of the fundamental extensive quantity thus forming an intensive quantity is often based on the norming extensive quantity to not change significantly in the attainable region in which the process operates. Probably the most common example is the volume. Constant volumes and constant densities are frequently applicable assumptions as the neglected nonlinearity is often very mild.

Let $\underline{\mathbf{q}}^b$ be the vector of norming extensive quantities with each element referring to the respective loop. The assumption is then constant norming quantities in each loop. Thus:

$$\frac{d\underline{\mathbf{q}}^b}{dt} = \underline{\mathbf{0}}. \quad (4)$$

and use it to slightly generalise the model (2):

$$\frac{d\underline{\xi}_I^b}{dt} = \left(\sum_r \underline{\mathbf{A}}_r \hat{\underline{\mathbf{q}}}_I^b + \underline{\mathbf{s}}_e \hat{q}_{e|P}^b \right) \underline{\xi}_I + \underline{\mathbf{b}}_F q_{F|}^b \xi_F.$$

Here the norming, constant extensive quantities have been wrapped into a diagonal matrices $\underline{\underline{\mathbf{q}}}_I^b$ and $\underline{\underline{\mathbf{q}}}_F^b$. With the assumption (4) this yields:

$$\underline{\underline{\mathbf{q}}}_I^b \frac{d\underline{\xi}_I}{dt} = \left(\sum_r \underline{\mathbf{A}}_r \hat{\underline{\mathbf{q}}}_I^b + \underline{\mathbf{s}}_e \hat{q}_{e|P}^b \right) \underline{\xi}_I + \underline{\mathbf{b}}_F q_{F|}^b \xi_F,$$

The assumption (4) has further the consequence that the flows of the extensive quantity \hat{q}^b in the individual recycle loops are the same and that the inflow is identical to the outflow: $\hat{q}_{i-1|i}^b = \hat{q}_{i|i+1}^b =: \hat{q}_r^b$ for all i in loop r and, $\hat{q}_{F|}^b = \hat{q}_{e|P}^b =: \hat{q}_E^b$. For simplicity reasons, we further assume that all capacitive elements in the plant are of equal size when the capacity is measured in the quantity q . Thus $q_m^b := q_i^b$ for all i . These assumptions and the substitution of the consequently defined quantities simplifies the model to

$$\frac{d\underline{\xi}_I}{dt} = \left(\sum_r \frac{\hat{q}_r^b}{q_m^b} \underline{\mathbf{A}}_r + \frac{\hat{q}_E^b}{q_m^b} \underline{\mathbf{s}}_e \right) \underline{\xi}_I + \frac{\hat{q}_E^b}{q_m^b} \underline{\mathbf{b}}_F \xi_F,$$

The fractions of flows of extensive quantity and capacity of elements measured in the same extensive quantity are the inverse of the time constants associated with mixing in each element and the effect of the in- and outflow of to and from the plant. The inverse of these time constants can be interpreted as frequencies, in simple cases corner frequencies: $\nu_r := \frac{\hat{q}_r^b}{q_m^b}$, $\nu_E := \frac{\hat{q}_E^b}{q_m^b}$. The model is now cast in its final form:

$$\frac{d\underline{\xi}_I}{dt} = \left(\sum_r \nu_r \underline{\mathbf{A}}_r + \nu_E \underline{\mathbf{s}}_e \right) \underline{\xi}_I + \nu_E \underline{\mathbf{b}}_F \xi_F, \quad (5)$$

$$= \underline{\underline{\mathbf{A}}} \underline{\xi}_I + \underline{\underline{\mathbf{b}}} \xi_F. \quad (6)$$

Lumping : a First-Order Model

The idea of reducing the order is to lump all recycles into one big lump. The result of this lumping is a first-order differential equation, which under the same mild conditions as assumed before, is linear and can be readily integrated for simple inflow profiles, which change only the intensive properties of

the inflow. Similarly the detailed model can be integrated. The difference is the approximation error made when using the single-lump model instead of the model with the recycles for a given inflow profile in the intensive property of the feed stream.

Simply summing up all the small elements does the lumping, which mathematically is achieved by multiplying the extended version of equation (1) with the left null matrix of the matrix $\underline{\underline{A}}$, which is the transposed of a vector of ones \underline{e} of corresponding length :

$$\underline{e}^T \frac{d\mathbf{Q}_I}{dt} = \underline{e}^T \left(\sum_r \underline{\underline{A}}_r \hat{\mathbf{Q}}_I + \underline{\underline{B}}_E \hat{\mathbf{Q}}_E \right).$$

This operation eliminates all internal flows. This result can also be derived by recognising that column sum of the recycle matrices $\underline{\underline{A}}_r$ is null. Defining the lumped quantity: $\bar{Q}_I^a := \underline{e}^T \mathbf{Q}_I$. Thus $\frac{d\bar{Q}_I^a}{dt} = \underline{e}^T \underline{\underline{B}}_E \hat{\mathbf{Q}}_E$. Again, the intensive quantity is of interest. Thus we define the intensity for the lumped system in the same way as before: $\bar{\xi}_I := \frac{\bar{Q}_I^a}{q_I^b}$. Again assuming that the extensive quantity q_I^b does not change appreciably, and splitting the term with the matrix $\underline{\underline{B}}_E$ as before, the model is cast into a new form:

$$\frac{d\bar{\xi}_I}{dt} = \frac{\hat{q}_E^b}{q_I^b} \left(\underline{e}^T \underline{\underline{B}}_P \bar{\xi}_I + \underline{e}^T \underline{\mathbf{b}}_F \xi_F \right).$$

In the case of the single inflow, single outflow process, and defining the corner frequency $\bar{v} := \frac{\hat{q}_E^b}{q_I^b}$, which reduces to

$$\frac{d\bar{\xi}_I}{dt} = \bar{v} (-\bar{\xi}_e + \bar{\xi}_F). \quad (7)$$

This model describes the process still based on the recycle model because it uses the intensive state ξ_e , which can be obtained by integrating the recycle model (6). The observation, though, that at steady state all the internal intensities approach the same value, stimulates the idea of simply replacing intensity of the exit element with the averaged intensity $\bar{\xi}_I$. Introducing a new intensive variable, indicating with a $\tilde{\cdot}$ the approximation of ξ_I , results the final approximate first-order model:

$$\frac{d\tilde{\xi}_I}{dt} = \bar{v} (-\tilde{\xi}_I + \bar{\xi}_F). \quad (8)$$

Impulse Responses-A Comparison

A comparison of the impulse response of models provides, when plotted, an excellent visual measure for the fidelity of the models. Both, the impulse response of the recycle model and the lumped model are readily computed. Starting with the definition of the inflow change: $\xi_F(t) := \xi_F^o \delta(t - 0)$. The recycle model is to be integrated for the solution, assuming zero initial conditions:

$$\begin{aligned} \underline{\xi}_I(t) &:= v_E \int_0^t \underline{\underline{e}}^{\underline{\underline{A}}(t-\tau)} \underline{\mathbf{b}}_F \xi_F(\tau) d\tau, \\ &:= v_E \underline{\underline{e}}^{\underline{\underline{A}}t} \underline{\mathbf{b}}_F \xi_F^o. \end{aligned}$$

The intensity of the element where the outflow is

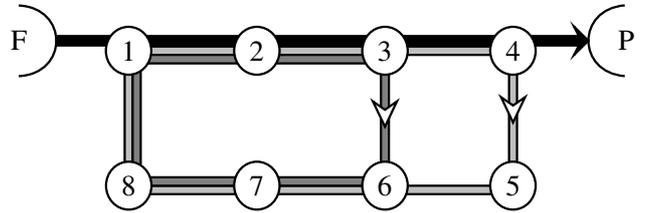


Figure 2: A sample plant with 8 lumps and three streams

connect is the e^h element in the solution vector. It is selected by multiplying the solution with the transposed of the e-selection vector, being zero except the e^h element, which is one. The such found intensity $\xi_e(t)$ is substituted into model (7):

$$\frac{d\bar{\xi}_I}{dt} = \bar{v} \left(-v_E \underline{\underline{c}}_e^T \underline{\underline{e}}^{\underline{\underline{A}}t} \underline{\mathbf{b}}_F \xi_F^o + \bar{\xi}_I(t) \right),$$

which needs to be integrated again:

$$\begin{aligned} \bar{\xi}_I(t) &= \bar{v} \left(-v_E \underline{\underline{c}}_e^T \int_0^t \underline{\underline{e}}^{\underline{\underline{A}}\tau} d\tau \underline{\mathbf{b}}_F \xi_F^o + \int_0^t \bar{\xi}_I(\tau) d\tau \right), \\ &= \bar{v} \left(-v_E \underline{\underline{c}}_e^T \underline{\underline{A}}^{-1} \left(\underline{\underline{e}}^{\underline{\underline{A}}t} - \mathbf{I} \right) \underline{\mathbf{b}}_F + 1 \right) \xi_F^o. \end{aligned}$$

The solution for the approximate model (8) is simple: $\tilde{\xi}_I(t) = \bar{v} \underline{\underline{e}}^{-\bar{v}t} \cdot \xi_F^o$. Finally we can compute various errors for ex.: $e(t) := \bar{\xi}_I - \tilde{\xi}_I$. The attached plots, show the solutions for the two recycle process shown in Figure 2. The volumetric flows in the two recycles are 1, and the inflow, respective the outflow, is 0.1. The total volume of the plant is set to 1 and the internal volumes are all the same, thus the individual volume is 1/8 in this case, as there are 8 lumps all together.

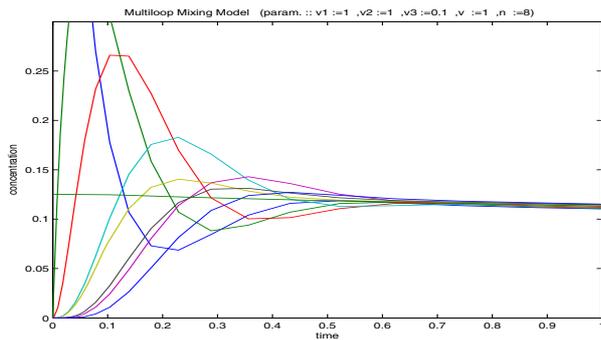


Figure 3: *Simulated impulse response of 8 equally sized tanks and a single-lumped approx.*

Plot 3 shows the impulse response of the 8 lumps, model 6, and the smooth middle one is the impulse response of the single lump approximation of model 7. Figure 4 finally shows the difference between the model (7) and the model and (8).

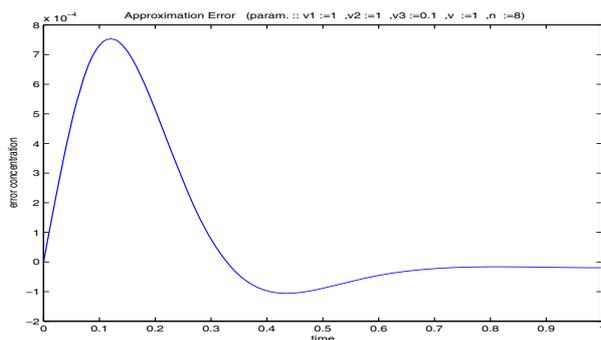


Figure 4: *Error between model 7 and 8*

Conclusions

The concise representation, as it was developed as part of our Modeller project ([7]) of process systems enables a generic analysis of such processes. The here-discussed recycle process is generic and not dependent of the nature of the sub-processes. The analysis also makes the different steps and assumptions nicely visible: 1) Split plant into fast and slow section. 2) Assume slow interaction between the fast and the slow section, thus limiting the spectrum of interaction and implicitly defining fast and slow. 3) In the long time scale one assumes fast internal dynamics, which results in uniform intensive

quantities inside the system. 4) Using the above result, all the internal dynamics can be lumped into one. 5) Notice: Time constants of the plant become explicitly visible once one transforms from the space of the conserved extensive quantities into the space of the conjugate intensive quantities.

Results published in the literature, such as [3] on special processes can be nicely generalised using the generic, physics-based representation as it is presented here and in [4] if event dynamic reactions are involved.

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