

Article

Extended Definition of Conversion and Reaction Extent for a Systematic Development of the Design Equations for Reactor Networks

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Abstract: The aim of this work is to present in a systematic way a novel general methodology to develop the design equations (heat and mass balances) for networks of ideal reactors, that is, *Plug-Flow Reactors* (PFRs) and *Continuous Stirred Tank Reactors* (CSTRs). In particular, after introducing the general definition of conversion to be used for reactor networks, several case studies of interest in chemical engineering are presented as topic-examples of application: (i) adiabatic-stage reactors with recycle, (ii) adiabatic-stage reactors with split, (iii) adiabatic-stage reactors intercooled by reactants and (iv) adiabatic-stage reactors with interstage distributed feed. More generally, the presented methodology can also be applied to develop the design equations for complex networks of interconnected reactors, not restricted to those considered in the present work. The motivation behind the present study lies in the fact that, to the best of our knowledge, a systematic development of the design equations of single reactors in reactor networks is currently missing in the open literature as well as in the reference textbooks of chemical reaction engineering and reactor design.

Keywords: reactor networks; design equations; conversion; reaction extent; ideal reactors



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1. Introduction

Nowadays, to increase the performance of existing production processes as well as to develop innovative and more efficient ones, there is a need to rethink the approach to the design of reaction units.

Chemical reactors represent the core of the production processes, in which lower-value raw materials are upgraded to higher-value products. Such a transformation occurs through several steps that generally involve a number of complex chemical reactions, which most of the time would be convenient to carry out in different reactors to maximise selectivity, and are pointed out in the textbook of Ming et al. (2016) [1–3].

Moreover, the increasing interest in modular and compact micro-reactors in chemical, biochemical and pharmaceutical processes [3,4], as well as the related technological enhancements, including complex reactor configurations [5], make a question arise about the need to develop a general design methodology for such systems.

The field of designing efficient reaction systems starting from complex reaction paths through more or less advanced techniques of *Mixed-Integer Non-Linear Programming* (MINLP) is called *Attainable Region Theory*, whose main topic is to deal with complex reactor networks [3]. MINLP techniques are necessary because the design of an optimal reactor system involves not only real variables like conversion, yields and selectivities but also integer variables like the number of reactors and their position in the network. A few literature examples of efficient reactor networks are reported in Figure 1 [6].

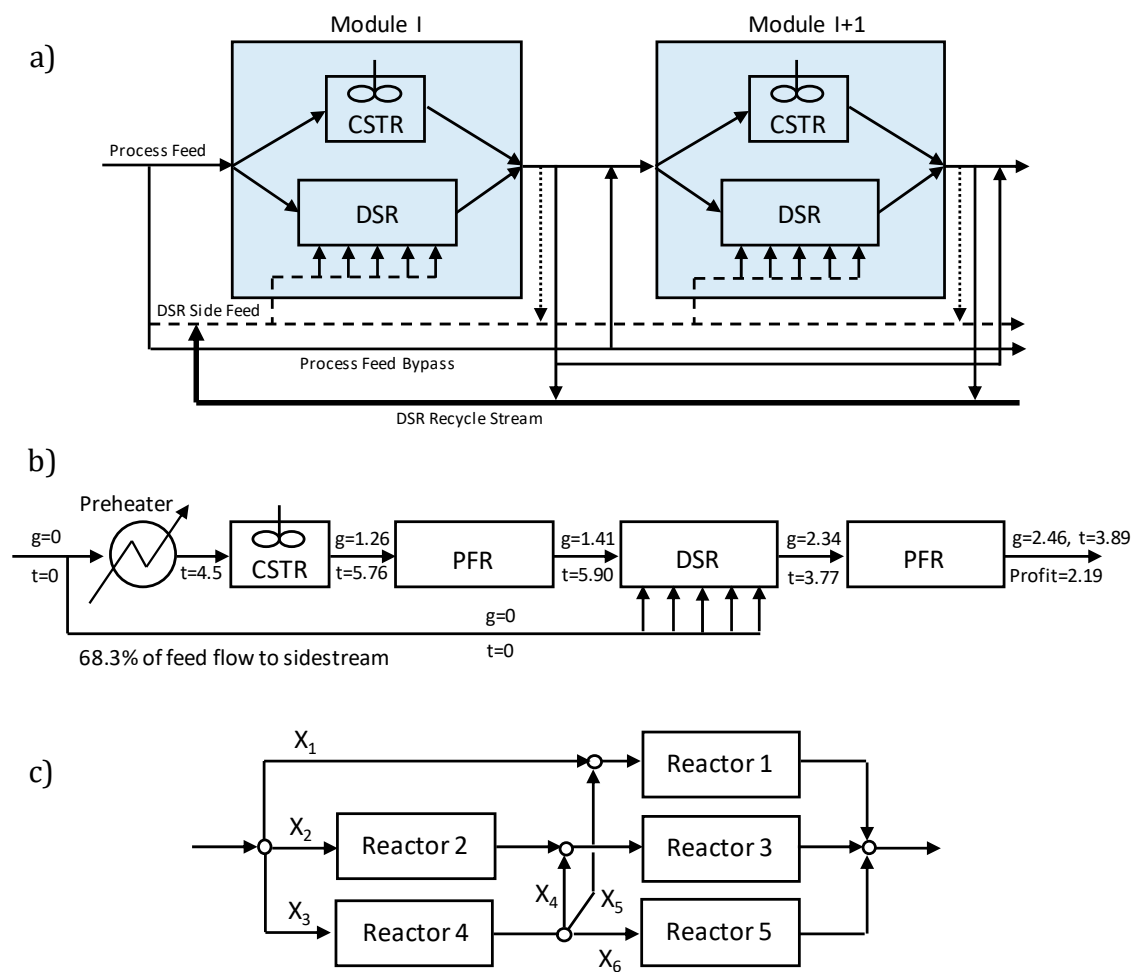


Figure 1. Examples of complex reactor networks from (a,b) Rooney and Biegler (2000) [5] and (c) Xie and Freund (2018) [7]. Rearranged with the permission of Elsevier.

Objectives and Motivations

The objective of the present work is to present in a systematic and general way the design methodology of complex reactor networks with ideal reactors operated in steady state, that is, *CSTRs* (*Continuous Stirred Tank Reactors*) and *PFRs* (*Plug-Flow Reactors*). The target readers are chemical and process engineers involved in the design and optimisation of chemical reactors, as well as scientists and students in their advanced courses who may need a systematic approach to the development and analysis of reactor networks.

The reason for presenting this work is based on the fact that there are currently no systematic and specific approaches dealing with writing the design equations of the single reactors of complex reactor networks in terms of conversion or, more generally, of reaction extents [1,4,7–53]. The extension of the present approach to non-ideal reactors or other types of reactors is straightforward.

To approach the design of reactor networks in a systematic way, we first generalise the concept of conversion as well as the concept of reaction extents in the case of multiple reactions. Then, we develop and report in detail the design equations—that is, mass and energy balances—for different key types of reactor networks.

For these purposes, the paper is organised to present and discuss the final equations directly in the body of the text, reporting the details of the systematic procedure in the corresponding appendices. This is performed to avoid weighing down the body of the work owing to the unavoidable presence of a high number of equations.

2. Methodology of the General Design Approach

The following sub-sections report the description of the main steps leading to the correct formalisation of the design equations, including a brief introduction to the reactor networks along with the general definition of conversion and reaction degrees.

2.1. Reactor Networks

A generic reactor network consists of a number of reactors and mix/split nodes appropriately connected to each other, whose connections represent the branches of the network (Figure 2).

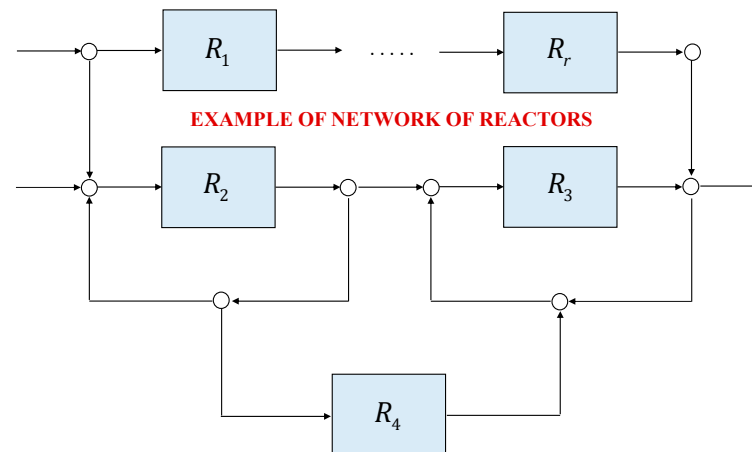


Figure 2. Example of a generic reactor network connected to each other in series/parallel through several oriented branches.

In this paper, we consider just the ideal PFRs and CSTRs, as all the other reactive systems can actually be obtained by appropriate modifications/combinations of them. Each reactor represents a reactive node, characterised by a single functioning point in the case of the CSTRs and by a continuous working profile in the case of the PFRs.

Based on *The Theory of Graphs* [43], a reactor network can be represented by a *directed graphs* since the particular orientation of the arrows connecting the nodes does matter in determining its performance since a change in the connection direction causes a change in the network's functioning.

By definition, the design equations of a device are relationships pairing mass, energy and momentum balances expressed in terms of convenient independent and dependent variables. In this work, time is not included in the independent variables, as we consider ideal reactors working in steady-state conditions. The independent variables represent a measure of the system size—usually volume, length, catalyst mass or catalytic area—whereas the dependent variables measure the extent of mass or molar flow rates, mass or molar fractions and similar.

In the description of this general approach, the momentum balance—which determines the fluid dynamics of the stream in the reactor—will not be considered because the velocity field is already fixed in the ideal PFRs and CSTRs by hypothesis. Furthermore, for pressure, the well-known Ergun equation (or its various modifications) can be satisfactorily used to calculate the pressure drop.

Depending on whether we know the values of the dependent variables or the independent ones, we have to address:

(i) a *design problem*—in which the dependent variables are known (in terms of final performance, conversion or a general productivity index) and the independent variables need to be evaluated;

(ii) a *verification problem*—in which the independent variables are known in terms of system size (volume, catalyst mass, catalyst volume, etc.) and the dependent ones need to be evaluated and compared to the target performances.

In general, we can write the mass balances either in terms of the flow rate of the species or in terms of reaction extents as well as conversion or yield in the case of a single reaction. In the following sections, the following notation is adopted to indicate the characteristic number of network objects along with the corresponding indices:

- $\{n, i\} = \{\text{Number of Species, Related Index}\};$
- $\{m, j\} = \{\text{Number of Reactions, Related Index}\};$
- $\{r, k\} = \{\text{Number of Reactors, Related Index}\};$
- $\{b, l\} = \{\text{Number of Network Branches, Related Index}\}.$

2.2. General Extension of the Definition of Conversion

To approach the reactor network design in a systematic way, we introduce the extension of the general definition of conversion (x_A), which from now on refers to the limiting reactant, indicated by the subscript 'A'.

In particular, starting from considering that each l -th branch of the network is provided with a certain non-null conversion value, we extend the general definition of conversion by taking the working conditions occurring in that branch in the absence of reaction as the reference state based on which conversion is defined (Equations (1) and (2)):

$$\text{Conversion}_A^{(l\text{th branch})} \equiv \frac{\left\{ \begin{array}{c} \text{Flow Rate of A in} \\ \text{the Non - Reactive} \\ \text{Network} \end{array} \right\}^{(l\text{th branch})} - \left\{ \begin{array}{c} \text{Flow Rate of A} \\ \text{in the Reactive} \\ \text{Network} \end{array} \right\}^{(l\text{th branch})}}{\left\{ \begin{array}{c} \text{Flow Rate of A in} \\ \text{the Non - Reactive} \\ \text{Network} \end{array} \right\}^{(l\text{th branch})}} \quad (1)$$

$$x_A^{(l)} \equiv \frac{F_A^{*(l)} - F_A^{(l)}}{F_A^{*(l)}} \Rightarrow F_A^{(l)} = F_A^{*(l)} (1 - x_A^{(l)}) \quad (2)$$

where F_A is the molar flow rate of the species A and the asterisk '*' indicates the molar flow rate of A in the l -th branch of the network (superscripted) in the absence of reaction.

In the case of multiple reactions, it is not possible to write the design equations in terms of the sole conversion since we have as many design variables as many independent reactions. To face this problem, analogously to what is performed in the single-reaction case, we can use the molar reaction extents (ξ_j , Equation (3)), which are design parameters measuring the extent to which each reaction proceeds forward in each l -th branch of the network.

$$F_A^{(l)} \equiv F_A^{*(l)} + \sum_{j=1}^m \nu_{Aj} \xi_j^{(l)} \quad (3)$$

In cases where it is convenient to work with dimensionless parameters instead of using ξ_j , which have units of a molar flow rate, we can define the here-called *reaction degrees* x_j in the generic l -th branch of the network as the ratio of the reaction extents ξ_j and the molar flow rate of the key-reactant (A) in the same branch of the network in the absence of reaction (Equation (4)).

$$x_j^{(l)} \equiv \frac{\xi_j^{(l)}}{F_A^{*(l)}} \quad (4)$$

Such a definition is suggested by the form of Equation (3) and is chosen in analogy with the definition of conversion (see Equation (2)). By definition, the parameters x_j can also assume values higher than unity.

For the purposes of the present paper, we will focus on the single-reaction case, which implies the use of the conversion to express the mass balances. The extension to the multi-reaction system is straightforward.

Once given the general definition of conversion, we can express the molar flow rates of the species in terms of the conversion itself as follows (Equation (5)):

$$\begin{aligned} F_A^{(l)} &= F_A^{*(l)} (1 - x_A^{(l)}) \\ F_i^{(l)} &= F_A^{*(l)} \left(\theta_i + \frac{\nu_i}{a} x_A^{(l)} \right) \\ \theta_i &\equiv \frac{F_i^{(l)}}{F_A^{*(l)}}, \quad a = -\nu_A > 0 \end{aligned} \quad (5)$$

where θ_i is the feed ratio of the i -th species, defined with respect to the key-reactant A. We remind you that the stoichiometric coefficient of the limiting species A, ν_A , is negative.

It is necessary to put in evidence that, in the absence of reaction and in the presence of a single feed to the network, the feed ratio θ_i is the same in all the branches of the network, as the mixing and split nodes do not provide a selective separation among species.

On the contrary, in the case of separate feed streams, like in the distributed-feed system analysed in Section 3, the feed ratios θ_i evaluated at the beginning of the network are different from those in the various network branches.

We underline that the here-presented general definition of conversion implies a paradigm change. In fact, the stoichiometric table, which represents the mass balances for all the species involved in the system, has to be written not between the inlet and outlet of the reactor but “between” the non-reactive and reactive cases on each l -th branch of the network (see Table 1).

Table 1. General stoichiometric table written on the l -th branch of the network.

Stoichiometric Table on the l -th Branch of the Network		
Species i	Non-Reactive Case	Reactive Case
A (limiting species)	$F_A^{*(l)}$	$F_A^{(l)} = F_A^{*(l)} (1 - x_A^{(l)})$
$\vdots$	$\vdots$	$\vdots$
i	$F_i^{*(l)} = F_A^{*(l)} \theta_i$	$F_i^{(l)} = F_A^{*(l)} \left(\theta_i + \frac{\nu_i}{a} x_A^{(l)} \right)$
$\vdots$	$\vdots$	$\vdots$
Z	$F_Z^{*(l)} = F_A^{*(l)} \theta_Z$	$F_Z^{(l)} = F_A^{*(l)} \left(\theta_Z + \frac{\nu_Z}{a} x_A^{(l)} \right)$

It is easy to demonstrate that the general definition of conversion reported in Equations (1) and (2) includes the definition of conversion in single reactors as well as in the simplest reactor networks, that is, a series of reactors and reactors in parallel, as reported in Sections 2.3.1 and 2.3.2. Figure 3 shows the general algorithm to systematically obtain the design equations of the reactors in a network.

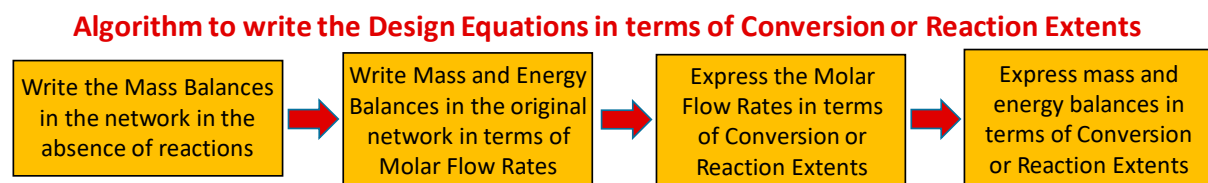


Figure 3. Systematic procedure to write the design equations for a reactor network.

2.3. Approach Validation Using Simple Reactor Networks

In this section, we report our general approach applied to the simplest reactor network, that is, a series of reactors and reactors placed in parallel in order to show that such networks can be seen as particular cases of more general configurations.

2.3.1. Series of Reactors in a Row

As for the series of reactors, the reference flow rate of A corresponds to the flow rate at the beginning of the series, and as in the non-reaction case, all the flow rates entering and exiting the reactors are equal (Figure 4).

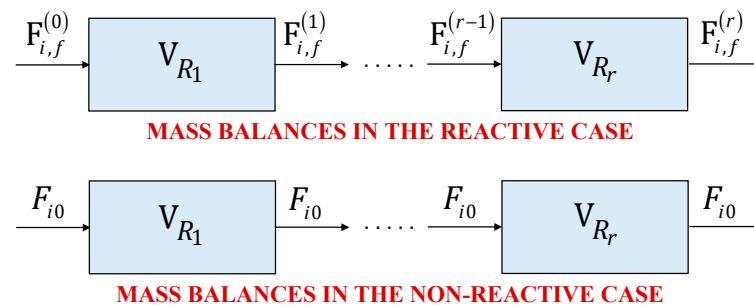


Figure 4. Scheme of reactors in series in reactive and no-reaction cases.

Using the general definition stated in Equations (1) and (2), we obtain the conversion in the l -th branch (Equation (6)), which is found to be equivalent to the conventional expression reported in almost all the reference textbooks on reactor design (see, e.g., [1,9–33]).

$$x_{A,f}^{(l)} \equiv \frac{F_{A,f}^{*(l)} - F_{A,f}^{(l)}}{F_{A,f}^{*(l)}} = \frac{F_{A0} - F_{A,f}^{(l)}}{F_{A0}} \quad (6)$$

$$\Downarrow$$

$$F_{A,f}^{(l)} = F_{A0} (1 - x_{A,f}^{(l)})$$

2.3.2. Reactors in Parallel

As for reactors in parallel (Figure 5), using the same procedure, we obtain the expressions reported in Equation (7).

$$x_{A,f}^{(l)} \equiv \frac{F_{A,f}^{*(l)} - F_{A,f}^{(l)}}{F_{A,f}^{*(l)}} = \frac{S_l F_{A0} - F_{A,f}^{(l)}}{S_l F_{A0}} \Rightarrow F_{A,f}^{(l)} = S_l F_{A0} (1 - x_{A,f}^{(l)}) \quad (7)$$

$$x_A = \frac{F_{A0} - F_A}{F_{A0}} \Rightarrow F_A = F_{A0} (1 - x_A)$$

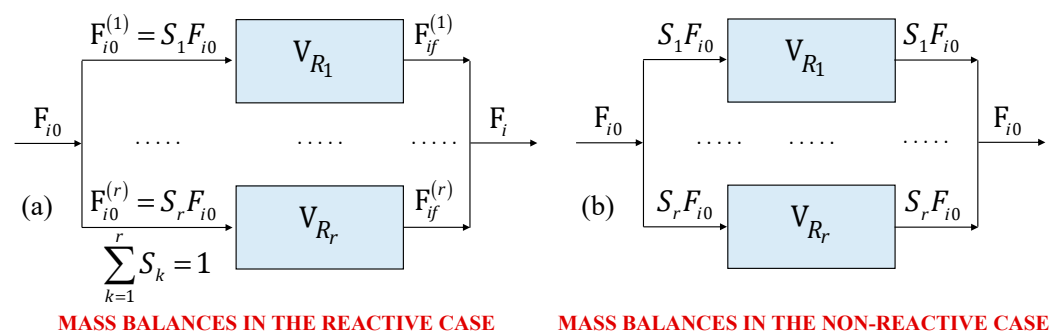


Figure 5. Scheme of reactors in parallel in (a) reactive and (b) no-reaction cases.

From the mass balance on the outlet mixing node, we can demonstrate that the optimal working conditions for reactors in parallel correspond to having the same conversion in all the outlet branches, as demonstrated by some algebraic calculations in Equations (8)–(10):

$$\begin{aligned} \sum_{l=1}^r F_{Af}^{(l)} &= \sum_{l=1}^r S_l F_{A0} (1 - x_{Af}^{(l)}) = F_A = F_{A0} (1 - x_A) \\ \sum_{l=1}^r S_l (1 - x_{Af}^{(l)}) &= (1 - x_A) \Rightarrow \underbrace{\sum_{l=1}^r S_l}_{=1} - \sum_{l=1}^r S_l x_{Af}^{(l)} = (1 - x_A) \end{aligned} \quad (8)$$

$$\sum_{l=1}^r S_l x_{Af}^{(l)} = x_A, \max_{\underline{S}} x_A \Rightarrow \frac{\partial x_A}{\partial S_l} = 0 \quad (9)$$

$$\begin{aligned} \frac{\partial x_A}{\partial S_l} &= \frac{\partial}{\partial S_l} \left(\sum_{l=1}^r S_l x_{Af}^{(l)} \right) = \frac{\partial}{\partial S_l} \left(\sum_{l=1}^{r-1} S_l x_{Af}^{(l)} + S_r x_{Af}^{(r)} \right) \Rightarrow \\ \frac{\partial}{\partial S_l} \left[\sum_{l=1}^{r-1} S_l x_{Af}^{(l)} + \left(1 - \sum_{l=1}^{r-1} S_l \right) x_{Af}^{(r)} \right] &= x_{Af}^{(l)} - x_{Af}^{(r)} = 0 \Rightarrow \\ x_{Af}^{(l)} &= x_{Af}^{(r)} \end{aligned} \quad (10)$$

2.3.3. Adiabatic-Stage Reactors with Recycle (See Appendix A.2)

This configuration is already present in several textbooks on chemical reactor design (see, e.g., Levenspiel, 1999 [9]) and is considered here for validation purposes. Figure 6a,b show the scheme of a series of adiabatic-stage reactors with recycle along with the corresponding scheme in the absence of reaction.

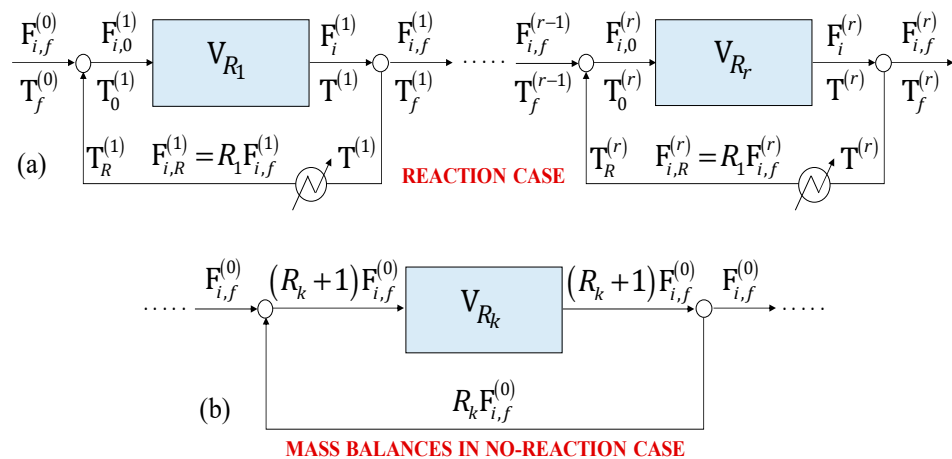


Figure 6. (a) Scheme of adiabatic-stage reactors with recycle (the position of the exchangers can be conveniently different based on the particular reactions considered) and (b) scheme of the generic k -th stage with explicit mass balance (in terms of molar flow rates) in the no-reaction case.

It is pointed out that we denote as “stage” the repeating unit of the series, consisting of a reactor along with the recycle stream. The subscript ‘ f ’ indicates the outlet of the stage to distinguish it from the outlet of reactor (i.e., the stream just before the split node). In fact, in this type of system, it is convenient to express the design equations as functions of the stage variables instead of those of the reactor.

Using the aforementioned extended definition of conversion, we can express the flow rates in the k -th branch of the reactor network as functions of conversions as follows (Equation (11), see Equation (A6) in the Appendix A):

$$\begin{aligned} F_{A,0}^{(k)} &= F_{A,0}^{*(k)} (1 - x_{A,0}^{(k)}) = (R_k + 1) F_{A,f}^{(0)} (1 - x_{A,0}^{(k)}) \\ F_A^{(k)} &= F_A^{*(k)} (1 - x_A^{(k)}) = (R_k + 1) F_{A,f}^{(0)} (1 - x_A^{(k)}) \end{aligned} \quad (11)$$

The mass balance on the mixing nodes leads to the following relation among inlet, outlet and stage conversions (Equation (12), see Equation (A8) in the Appendix A):

$$\begin{aligned} x_{A,0}^{(k)} &= \frac{1}{(R_k+1)} x_{A,f}^{(k-1)} + \frac{R_k}{(R_k+1)} x_{A,f}^{(k)} \\ x_A^{(k)} &= x_{A,f}^{(k)} \end{aligned} \quad (12)$$

Consequently, the mass balance on the k -th PFR is obtained as follows (Equation (13)):

$$\frac{V_{R_k}}{F_{A,f}^{(0)}} = (R_k + 1) \int_{\frac{1}{(R_k+1)} x_{A,f}^{(k-1)} + \frac{R_k}{(R_k+1)} x_{A,f}^{(k)}}^{x_{A,f}^{(k)}} \frac{dx_A}{(-r_A)} \quad (13)$$

whereas the mass balance on CSTR is (Equation (14)):

$$\frac{V_{R_k}}{F_{A,f}^{(0)}} = \frac{(x_{A,f}^{(k)} - x_{A,f}^{(k-1)})}{(-r_{A_k})} \quad (14)$$

As for the energy balance on the mixing nodes, the final resulting inlet temperature is found, as expected, to be a weighted average of both entering temperatures (Equation (15), see Equation (A17) in the Appendix A):

$$\begin{aligned} T_0^{(k)} &= \frac{1}{(R_k+1)} \left(\frac{\tilde{C}p_s + \Delta\tilde{C}p_A x_{A,f}^{(k-1)}}{\tilde{C}p_s + \Delta\tilde{C}p_A x_{A,0}^{(k)}} \right) T_f^{(k-1)} + \frac{R_k}{(R_k+1)} \left(\frac{\tilde{C}p_s + \Delta\tilde{C}p_A x_{A,f}^{(k)}}{\tilde{C}p_s + \Delta\tilde{C}p_A x_{A,0}^{(k)}} \right) T_f^{(k)} \\ T^{(k)} &= T_f^{(k)}, \Delta\tilde{C}p_A \equiv \frac{\Delta\tilde{C}p}{a} \end{aligned} \quad (15)$$

Under the hypothesis of negligible $\Delta\tilde{C}p_A$, the following relation is obtained (Equation (16), see Equation (A18) in the Appendix A):

$$T_0^{(k)} = \frac{1}{(R_k+1)} T_f^{(k-1)} + \frac{R_k}{(R_k+1)} T_f^{(k)} \quad (16)$$

The energy balance on the k -th PFR is (Equation (17), see Equation (A21) in the Appendix A):

$$\frac{dT}{dV} = \frac{(-\Delta\tilde{H}_{r,A})(-r_A)}{F_{A,f}^{(0)}(R_k+1)(\tilde{C}p_s + \Delta\tilde{C}p_A x_A)}, \Delta\tilde{H}_{r,A} \equiv \frac{\Delta\tilde{H}_r}{a} \quad (17)$$

As for the energy balance on the k -th CSTR, we can express it either in terms of stage conversions or temperatures (Equation (18), see Equation (A25) in the Appendix A):

$$(x_{A,f}^{(k)} - x_{A,f}^{(k-1)}) = (R_k + 1) \frac{\tilde{C}p_s (T^{(k)} - T_0^{(k)})}{(-\Delta\tilde{H}_{r,A})} = \frac{\tilde{C}p_s (T_f^{(k)} - T_f^{(k-1)})}{(-\Delta\tilde{H}_{r,A})} \quad (18)$$

Geometrical Interpretation of Mass Balance

In order to show the geometrical meaning of the integral form of the mass balance on *PFR* (Equation (13)), we obtain the k -th recycle ratio R_k and $(R_k + 1)$ as functions of the inlet and outlet conversions as follows (Equation (19)):

$$\begin{aligned} x_{A,0}^{(k)} &= \frac{1}{(R_k+1)} x_{A,f}^{(k-1)} + \frac{R_k}{(R_k+1)} x_{A,f}^{(k)} \\ R_k &= \frac{x_{A,f}^{(k-1)} - x_{A,0}^{(k)}}{x_{A,0}^{(k)} - x_{A,f}^{(k)}}, \quad R_k + 1 = \frac{x_{A,f}^{(k-1)} - x_{A,f}^{(k)}}{x_{A,0}^{(k)} - x_{A,f}^{(k)}} \end{aligned} \quad (19)$$

Substituting Equation (19) into Equation (13), Equation (20) is obtained, which can be interpreted geometrically as shown in Figure 7.

$$\frac{V_{R_k}}{F_{A,f}^{(0)}} = \frac{x_{A,f}^{(k)} - x_{A,f}^{(k-1)}}{x_{A,f}^{(k)} - x_{A,0}^{(k)}} \cdot \int_{x_{A,0}^{(k)}}^{x_{A,f}^{(k)}} \frac{dx_A}{(-r_A)} = \left(x_{A,f}^{(k)} - x_{A,f}^{(k-1)} \right) \cdot \left. \frac{1}{(-r_A)} \right|_{x_{A,0}^{(k)}}^{x_{A,f}^{(k)}} \quad (20)$$

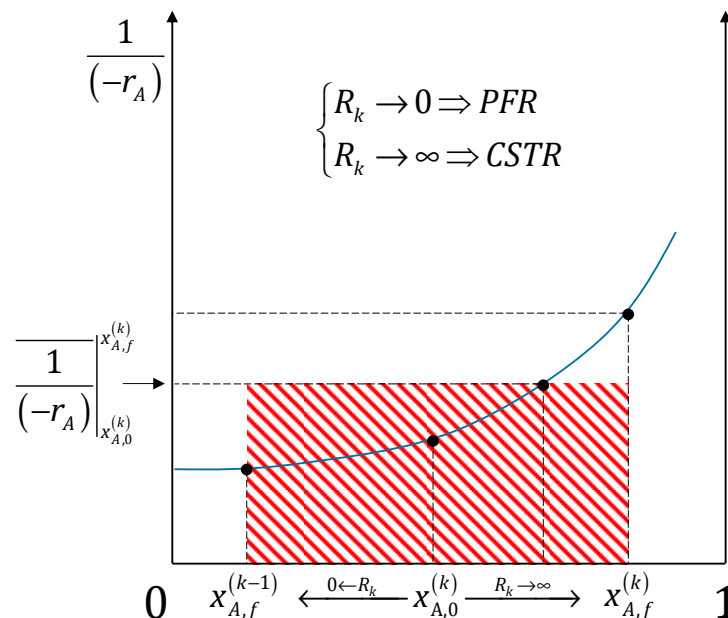


Figure 7. Sketch of the geometrical interpretation of the integral form of the design equation of *PFR* for a generic k -th reactor with recycle. The red area represents the ratio of the reactor volume and the flow rate of the limiting reactant A in that branch in the absence of reaction.

As already demonstrated in several reference books for a single reactor (see, e.g., ref. [9]), the V/F_{A0} ratio is found to be the product of the inlet–outlet conversion difference and the mean value of the reaction rate inverse calculated between inlet and outlet. It can also be noted that, in the limit value of $R_k = 0$, we obtain the usual design equation of *PFR*, whereas, for $R_k \rightarrow \infty$, the k -th reactor behaves as a perfectly mixed *CSTR*.

3. Application to Other Case Studies of Interest

To describe the systematic procedure for achieving the design equations for a reactor network, in the following sub-sections, we report the following three cases of a particular interest in chemical engineering, from which other possible and more complex cases can be constructed and analysed if required:

1. Adiabatic-Stage Reactors with Split;
2. Adiabatic-Stage Reactors Intercooled/Interheated by Reactants;
3. Adiabatic-Stage Reactors with Distributed Interstage Feed.

The main assumptions of the presented systematic procedure, along with the details of the intermediate calculation steps, are reported in the Appendix A.

3.1. Adiabatic-Stage Reactors with Split (See Appendix A.3)

The system considered here is similar to the previous one, with the important difference that now, in each stage, a partial split of feed is included in the inlet stream instead of a partial recycle of the outlet stream (Figure 8).

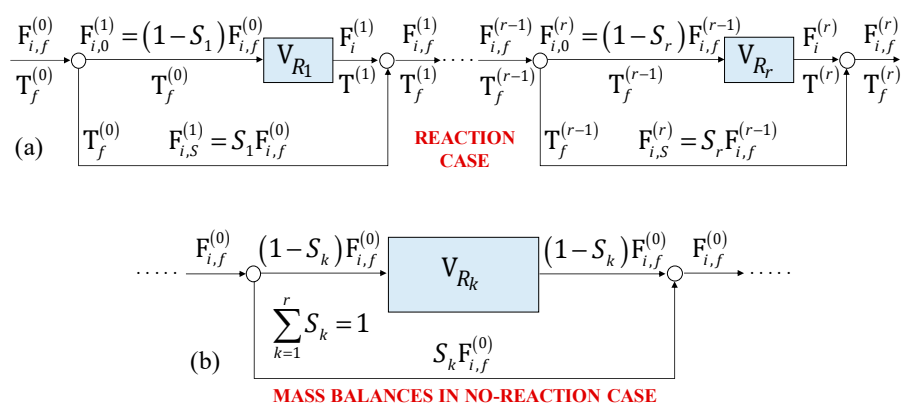


Figure 8. (a) Scheme of adiabatic-stage reactors with split and (b) scheme of the generic k -th stage with explicit mass balance (in terms of molar flow rates) in the no-reaction case.

The mass balance on the mixing nodes after the reactor is stated by the following relation among stage conversions (Equation (21), see Equation (A28) in the Appendix A):

$$x_A^{(k)} = \frac{1}{1 - S_k} x_{A,f}^{(k)} - \frac{S_k}{1 - S_k} x_{A,f}^{(k-1)} \quad (21)$$

The mass balance on the k -th PFR, expressed in terms of stage conversions, is obtained as follows (Equation (22), see Equation (A31) in the Appendix A):

$$\frac{V_{Rk}}{F_{A,f}^{(0)}} = (1 - S_k) \int_{x_{A,f}^{(k-1)}}^{\frac{1}{1-S_k} x_{A,f}^{(k)} - \frac{S_k}{1-S_k} x_{A,f}^{(k-1)}} \frac{dx_A}{(-r_A)} \quad (22)$$

whereas the mass balance on the k -th CSTR can be obtained in the following two forms (Equation (23), see Equations (A34) in the Appendix A):

$$\frac{V_{Rk}}{F_{A,f}^{(0)}} = (1 - S_k) \frac{(x_A^{(k)} - x_{A,0}^{(k)})}{(-r_{A_k})} = \frac{(x_{A,f}^{(k)} - x_{A,f}^{(k-1)})}{(-r_{A_k})} \quad (23)$$

As for the energy balance on the mixing nodes, it can be expressed as follows (Equation (24), see Equation (A36) in the Appendix A):

$$T^{(k)} = \frac{(\tilde{C}p_s + \Delta\tilde{C}p_A x_{A,f}^{(k)}) T_f^{(k)} - S_k (\tilde{C}p_s + \Delta\tilde{C}p_A x_{A,f}^{(k-1)}) T_f^{(k-1)}}{[(\tilde{C}p_s + \Delta\tilde{C}p_A x_{A,f}^{(k)}) - S_k (\tilde{C}p_s + \Delta\tilde{C}p_A x_{A,f}^{(k-1)})]} \quad (24)$$

In the hypothesis of negligible $\Delta\tilde{C}_p$, we obtain Equation (25) (see Equation (A37) in the Appendix A):

$$T^{(k)} = \frac{1}{(1-S_k)} T_f^{(k)} - \frac{S_k}{(1-S_k)} T_f^{(k-1)} \quad (25)$$

In combination with Equation (21), Equation (25) states the linearity of the working points of the streams at the mixing node in a $\{x_A \text{ vs. } T\}$ plane.

The differential form of the energy balance on the k -th PFR is obtained as follows (Equation (26), see Equation (A39) in the Appendix A):

$$\frac{dT}{dV} = \frac{(-\Delta\tilde{H}_{r,A})(-r_A)}{F_{A,f}^{(0)}(1-S_k)\left(\tilde{C}_p S + \frac{\Delta\tilde{C}_p}{a} x_A\right)} \quad (26)$$

whereas the energy balance on the k -th CSTR is (Equation (27), see Equations (A43) and (A44) in the Appendix A):

$$\left(x_{A,f}^{(k)} - x_{A,f}^{(k-1)}\right) = \frac{\tilde{C}_p S \left(T_f^{(k)} - T_f^{(k-1)}\right)}{(-\Delta\tilde{H}_{r,A})} \quad (27)$$

Geometrical Interpretation of Mass Balance

In order to show the geometrical meaning of the integral form of the mass balance on PFR (Equation (22)), we obtain the k -th split ratio and its complement to the unity as functions of the inlet and outlet conversions (Equation (28)):

$$\begin{aligned} x_{A,f}^{(k)} &= (1-S_k)x_A^{(k)} + S_k x_{A,f}^{(k-1)} \\ S_k &= \frac{x_A^{(k)} - x_{A,f}^{(k)}}{x_A^{(k)} - x_{A,f}^{(k-1)}}, \quad (1-S_k) = \frac{x_{A,f}^{(k)} - x_{A,f}^{(k-1)}}{x_A^{(k)} - x_{A,f}^{(k-1)}} \end{aligned} \quad (28)$$

Substituting Equation (28) into Equation (22), Equation (29) is obtained, which can be interpreted geometrically as shown in Figure 9.

$$\frac{V_{R_k}}{F_{A,f}^{(0)}} = \frac{x_{A,f}^{(k)} - x_{A,f}^{(k-1)}}{x_A^{(k)} - x_{A,f}^{(k-1)}} \cdot \int_{x_{A,f}^{(k-1)}}^{x_A^{(k)}} \frac{dx_A}{(-r_A)} = \left(x_{A,f}^{(k)} - x_{A,f}^{(k-1)}\right) \cdot \left. \frac{1}{(-r_A)} \right|_{x_{A,f}^{(k-1)}}^{x_A^{(k)}} \quad (29)$$

In particular, analogously to what was seen for the reactors with recycle, in this case, the V/F_{A0} ratio is found to be the product of the inlet–outlet conversion difference and the mean value of the reaction rate inverse calculated between the inlet and outlet conversion. It can also be noted that in the limit value of $S_k = 0$, we obtain the usual design equation of PFR, whereas for $S_k = 1$, there is a complete bypass of the reactor, which implies no reaction in the k -th reactor.

3.2. Adiabatic-Stage Reactors Intercooled/Interheated by Reactants (See Appendix A.4)

The third reactor network considered is a series of adiabatic reactors in which part of the feed of each reactor is split forward into the feed of the next one (Figure 10), with the main purpose of cooling down (for exothermic reactions) or heating up (for endothermic ones) the reactor inlet, thus pushing forward the thermodynamic equilibrium.

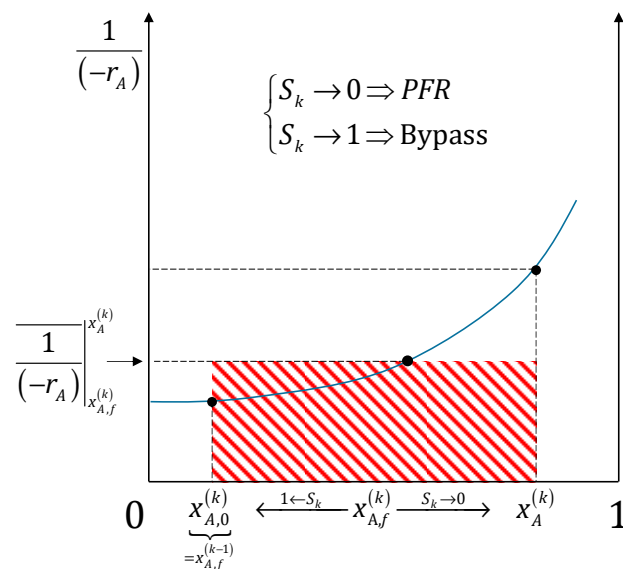


Figure 9. Sketch of the geometrical interpretation of the integral form of the design equation of the generic k -th PFR with split. The red area represents the ratio of the reactor volume and the flow rate of the limiting reactant A in that branch in the absence of reaction.

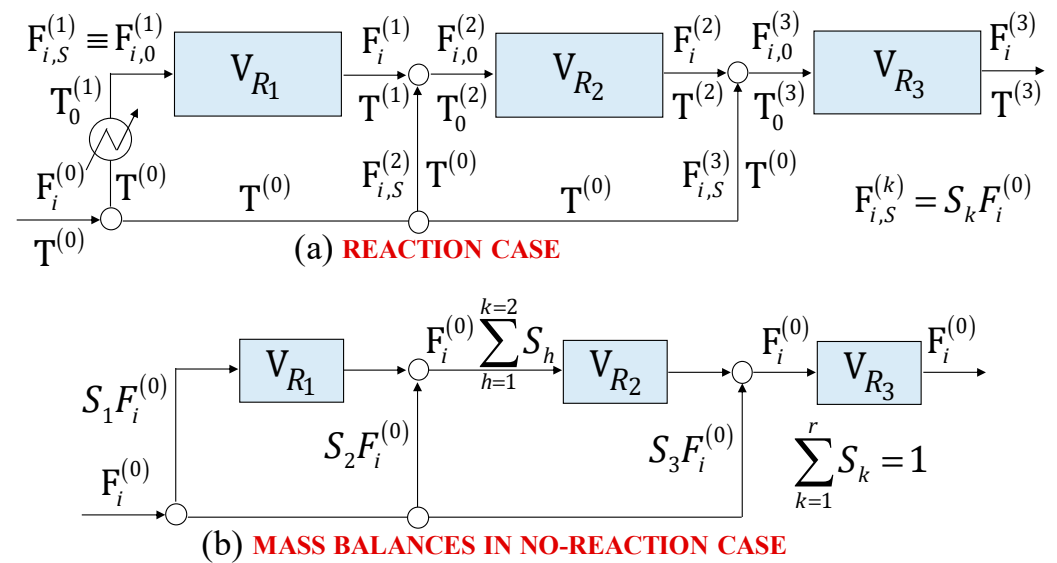


Figure 10. (a) Scheme of a series of adiabatic-stage reactors intercooled/interheated by reactants (example of three reactors) and (b) corresponding scheme of network with explicit mass balance (in terms of molar flow rates) in the no-reaction case.

The mass balance on the $(k - 1)$ -th mixing node is obtained as follows (Equation (30), see Equation (A48) in the Appendix A):

$$x_{A,0}^{(k)} = \frac{\sum_{h=1}^{k-1} S_h}{\sum_{h=1}^k S_h} x_A^{(k-1)} \Rightarrow x_{A,0}^{(k)} \Big|_{S_k=S} = \frac{k-1}{k} x_A^{(k-1)} \quad (30)$$

It can be noted that, in the case of equal split ratios, the inlet conversion is not a function of the split ratio itself but just of the number of splits. The mass balance

on the k -th PFR is obtained as follows (Equation (31), see Equations (A51) and (A52) in the Appendix A):

$$\frac{V_{R_k}}{F_A^{(0)}} = \left(\sum_{h=1}^k S_h \right) \cdot \int_{x_{A,0}^{(k)} = \frac{\sum_{h=1}^{k-1} S_h}{\sum_{h=1}^k S_h} x_A^{(k-1)}}^{x_A^{(k)}} \frac{dx_A}{(-r_A)} \quad (31)$$

$$\left. \frac{V_{R_k}}{F_A^{(0)}} \right|_{S_k=S} = kS \cdot \int_{x_{A,0}^{(k)} = \frac{k-1}{k} x_A^{(k-1)}}^{x_A^{(k)}} \frac{dx_A}{(-r_A)_k}$$

The total volume of the series is the sum of all reactor volumes or the series, as reported in Equation (32):

$$\frac{V_{RT}}{F_A^{(0)}} = \sum_{k=1}^r \frac{V_{R_k}}{F_A^{(0)}} = \sum_{k=1}^r \left\{ kS \cdot \int_{x_{A,0}^{(k)} = \frac{k-1}{k} x_A^{(k-1)}}^{x_A^{(k)}} \frac{dx_A}{(-r_A)} \right\} \quad (32)$$

The mass balance on the k -th CSTR is reported in Equation (33) (see Equation (A55) in the Appendix A):

$$\frac{V_{R_k}}{F_A^{(0)}} = \frac{\left[\left(\sum_{h=1}^k S_h \right) x_A^{(k)} - \left(\sum_{h=1}^{k-1} S_h \right) x_A^{(k-1)} \right]}{(-r_A)|_{R_k}} \quad (33)$$

$$\left. \frac{V_{R_k}}{F_A^{(0)}} \right|_{S_k=S} = S \frac{\left[kx_A^{(k)} - (k-1)x_A^{(k-1)} \right]}{(-r_A)|_{R_k}}$$

As for the energy balance on the mixing nodes, we obtain the following relations among temperatures (Equation (34), see Equation (A59) in the Appendix A):

$$T_0^{(k)} = \frac{\left(\sum_{h=1}^{k-1} S_h \right) [\tilde{C}p_S + x_A^{(k-1)} \Delta \tilde{C}p_A]}{\left(\sum_{h=1}^k S_h \right) [\tilde{C}p_S + x_{A,0}^{(k)} \Delta \tilde{C}p_A]} T^{(k-1)} + \frac{S_k \tilde{C}p_S}{\left(\sum_{h=1}^k S_h \right) [\tilde{C}p_S + x_{A,0}^{(k)} \Delta \tilde{C}p_A]} T^{(0)} \quad (34)$$

Under the hypothesis of constant enthalpy of reaction ($\Delta \tilde{C}p_A \approx 0$), the following simplified expressions are obtained (Equation (35), see Equation (A60) in the Appendix A):

$$T_0^{(k)} = \frac{\left(\sum_{h=1}^{k-1} S_h \right)}{\left(\sum_{h=1}^k S_h \right)} T^{(k-1)} + \frac{S_k}{\left(\sum_{h=1}^k S_h \right)} T^{(0)} \quad (35)$$

$$\left. T_0^{(k)} \right|_{S_k=S} = \frac{k-1}{k} T^{(k-1)} + \frac{1}{k} T^{(0)}$$

Taking into account the expression previously reported for the conversion in Equation (30), we can observe a linear functionality between conversion and temperature on the mixing nodes. However, it is stressed that such a linearity holds only if the enthalpy of the reaction can be considered constant.

As for the energy balance on the k -th PFR, it assumes the following form (Equation (36), see Equation (A62) in the Appendix A):

$$\begin{cases} \frac{dT}{dV} = \frac{(-\Delta\tilde{H}_{r,A})(-r_A)}{\left(\sum_{h=1}^k S_h\right) F_A^{(0)}(\tilde{C}p_S + \Delta\tilde{C}p_A x_A)} \\ T(V_k = 0) = T_0^{(k)} \end{cases} \quad (36)$$

which becomes Equation (37) in the case of an equal split ratio (see Equation (A63) in the Appendix A):

$$\begin{cases} \left. \frac{dT}{dV} \right|_{S_k=S} = \frac{(-\Delta\tilde{H}_{r,A})(-r_A)}{kS F_A^{(0)}(\tilde{C}p_S + \Delta\tilde{C}p_A x_A)} \\ T(V_k = 0) = T_0^{(k)} \end{cases} \quad (37)$$

The energy balance on the k -th CSTR (Equation (38), see Equations (A64) and (A65) in the Appendix A):

$$x_A^{(k)} = \frac{\tilde{C}p_S}{\Delta\tilde{H}_{r,A}^0(T^{(k)})} (T_0^{(k)} - T^{(k)}) + \frac{\Delta\tilde{H}_{r,A}^0(T_0^{(k)})}{\Delta\tilde{H}_{r,A}^0(T^{(k)})} x_{A,0}^{(k)} \quad (38)$$

In the case of constant enthalpy of reaction, Equation (38) can be simplified as follows (Equation (39), see Equation (A66) in the Appendix A):

$$\left[x_{A,0}^{(k)} - x_A^{(k)} \right] = \frac{\tilde{C}p_S}{-\Delta\tilde{H}_{r,A}} (T_0^{(k)} - T^{(k)}) \quad (39)$$

where the expressions previously obtained for $x_{A,0}^{(k)}$ and $T_0^{(k)}$ can be used to express the energy balance in terms of just outlet parameters, that is, $x_A^{(k)}$, $T^{(k)}$, $x_A^{(k-1)}$ and $T^{(k-1)}$.

3.3. Adiabatic-Stage Reactors with Distributed Interstage Feed (See Appendix A.5)

The last system considered in this analysis is depicted in Figure 11a. In particular, it involves the distributed feed of one component along a series of adiabatic reactors, with insertion in a mixing node located between two consecutive reactors. Such an interstage distributed feed can be used, for example, when the reaction rate is favoured by a low concentration of reactants and/or in the case of highly exothermic/endothermic reactions, for better and more efficient temperature control.

It must be highlighted that, in principle, the distributed stream, which we have considered here to be composed of a single species, can actually be composed of more than one species. However, the design equations related to the latter case can be easily obtained as a straightforward extension of the former one.

The scheme with the mass balance in the absence of reaction is reported as usual to express the flow rates as functions of conversion (Figure 11b). To obtain the design equations for this system, we suppose that species A is the key limiting species and the other reactants are in excess. Therefore, the feed of species A is distributed along the series at the mixing nodes placed between the inlet and outlet of two consecutive reactors.

The mass balance on the k -th mixing node is obtained as follows (Equation (40), see Equations (A69) in the Appendix A):

$$x_{A,0}^{(k)} = \frac{\sum_{h=1}^{k-1} S_h}{\sum_{h=1}^k S_h} x_A^{(k-1)} = \frac{k-1}{k} x_A^{(k-1)} \Big|_{S_k=S} \quad (40)$$

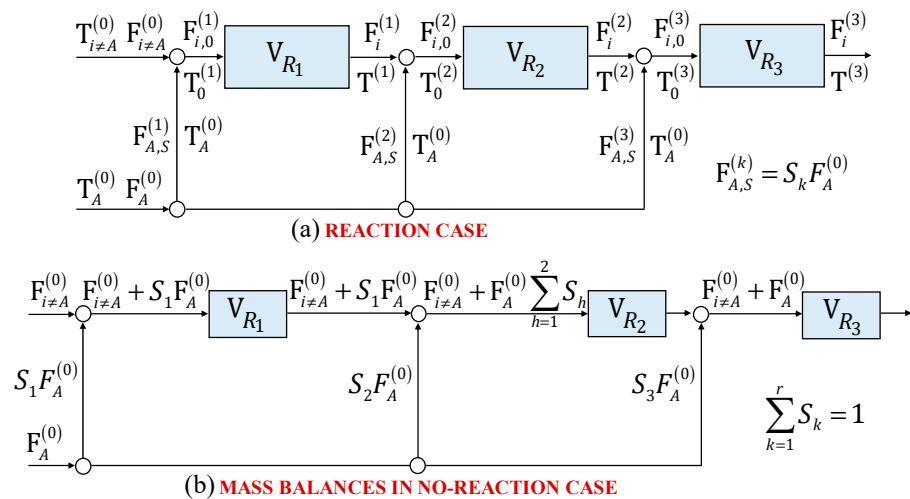


Figure 11. (a) Scheme of a series of adiabatic-stage reactors (example of three reactors) with the feed of one species distributed between two consecutive reactors and (b) corresponding scheme of network with explicit mass balance (in terms of molar flow rates) in the no-reaction case.

In Equation (40), we also report the particular case in which all the split ratios are the same, where it can be observed that the inlet conversion of the k -th reactor depends on the number of splits as well as on the conversion exiting the preceding reactor. All these expressions are needed to obtain the design equations for PFR and CSTR in terms of conversion.

As for the mass balance of the generic species $i \neq A$, which is required for the energy balance (see next sub-section), we first need to write down the molar flow rate of the generic species as a function of conversion, recalling the definition of the feed ratio $\theta_i^{(l)}$ on the l -th branch of the network in the absence of reaction and its relation with the feed ratio θ_i at the beginning of the network (Equation (41)):

$$\theta_i^{(l)} \equiv \frac{F_i^{*(l)}}{F_A^{*(l)}}, \quad \theta_i \equiv \frac{F_i^{*(0)}}{F_A^{*(0)}} = \frac{F_i^{(0)}}{F_A^{(0)}} \quad (41)$$

$$F_i^{(l)} = F_A^{*(l)} \left[\theta_i^{(l)} + \frac{v_i}{a} x_A^{(l)} \right], \quad F_A^{(l)} = F_A^{*(l)} (1 - x_A^{(l)})$$

In fact, in this particular network configuration, the quantities θ_i are different from $\theta_i^{(k)}$, since the ratio between the generic species i and the limiting species A in the absence of reaction is not the same in all network branches because of the partial insertion of the initial split flow rate in each reactor inlet stream.

As we wish to work with the quantities θ_i instead of $\theta_i^{(k)}$ because they are known and fixed at the inlet of the network, we can express such a relation starting directly from their respective definitions (Equation (42)):

$$\theta_i^{(k)} = \frac{F_i^{*(k)}}{F_A^{*(k)}} = \begin{cases} 1, & i = A \\ \frac{F_A^{*(0)} \theta_i}{F_A^{*(0)} \sum_{h=1}^k S_h} = \frac{\theta_i}{\sum_{h=1}^k S_h}, & i \neq A \end{cases} \quad (42)$$

$$F_{i \neq A}^{*(k)} = \theta_{i \neq A}^{(k)} F_A^{*(k)} = \frac{\theta_{i \neq A}}{\sum_{h=1}^k S_h} F_A^{*(k)}$$

Therefore, by writing down the mass balance at the mixing nodes for a generic species i different from the limiting one A , we obtain Equation (43), in which we remind that the species i_s are not contained in the split branches $F_{A,S}^k$:

$$\begin{aligned} F_{i \neq A}^{(0)} &= F_{i \neq A,0}^{(1)} \\ F_{i \neq A}^{(1)} &= F_{i \neq A,0}^{(2)} \\ &\dots \\ F_{i \neq A}^{(k-1)} &= F_{i \neq A,0}^{(k)} \end{aligned} \quad (43)$$

To prove the consistency of the definitions used in Equation (41), we express Equation (43) in terms of conversion, expecting to reach the same expressions as those previously obtained in Equation (40). The result of this checking is reported in Equations (44) and (45), which just state the full consistency of the expression reported above.

$$\begin{aligned} 0 &= 0 \text{ (Mix node 1, trivial : no conversion yet)} \\ F_A^{*(1)} \left[\theta_{i \neq A}^{(1)} + \frac{v_i}{a} x_A^{(1)} \right] &= F_{A,0}^{*(2)} \left[\theta_{i \neq A,0}^{(2)} + \frac{v_i}{a} x_{A,0}^{(2)} \right] \\ &\dots \\ F_A^{*(k-1)} \left[\theta_{i \neq A}^{(k-1)} + \frac{v_i}{a} x_A^{(k-1)} \right] &= F_A^{*(k)} \left[\theta_{i \neq A,0}^{(k)} + \frac{v_i}{a} x_{A,0}^{(k)} \right] \end{aligned} \quad (44)$$

$$\begin{aligned} \theta_{i \neq A}^{(k-1)} &= \frac{\theta_{i \neq A}}{\sum_{h=1}^{k-1} S_h}, \quad \theta_{i \neq A,0}^{(k)} = \frac{\theta_{i \neq A}}{\sum_{h=1}^k S_h} \\ F_A^{*(k-1)} &= F_A^{(0)} \sum_{h=1}^{k-1} S_h, \quad F_{A,0}^{*(k)} = F_A^{(0)} \sum_{h=1}^k S_h \\ F_A^{(0)} \sum_{h=1}^{k-1} S_h \left[\frac{\theta_{i \neq A}}{\sum_{h=1}^{k-1} S_h} + \frac{v_i}{a} x_A^{(k-1)} \right] &= F_A^{(0)} \sum_{h=1}^k S_h \left[\frac{\theta_{i \neq A}}{\sum_{h=1}^k S_h} + \frac{v_i}{a} x_{A,0}^{(k)} \right] \\ \left[\theta_{i \neq A} + \sum_{h=1}^{k-1} S_h \frac{v_i}{a} x_A^{(k-1)} \right] &= \left[\theta_{i \neq A} + \sum_{h=1}^k S_h \frac{v_i}{a} x_{A,0}^{(k)} \right] \\ x_{A,0}^{(k)} &= \frac{\sum_{h=1}^{k-1} S_h}{\sum_{h=1}^k S_h} x_A^{(k-1)} \end{aligned} \quad (45)$$

As for the mass balance on the k -th PFR, it is reported in Equation (46) for both variable and equal split ratios (see Equations (A72) and (A73) in the Appendix A):

$$\begin{aligned} \frac{V_{R_k}}{F_A^{(0)}} &= \left(\sum_{h=1}^k S_h \right) \int_{x_A^{(k-1)}}^{x_A^{(k)}} \frac{dx_A}{(-r_A)_{R_k}} \\ &\quad \frac{\sum_{h=1}^{k-1} S_h}{\sum_{h=1}^k S_h} x_A^{(k-1)} \\ \frac{V_{R_k}}{F_A^{(0)}} \Big|_{S_k=S} &= kS \int_{x_A^{(k-1)}}^{x_A^{(k)}} \frac{dx_A}{(-r_A)_{R_k}} \end{aligned} \quad (46)$$

The mass balance on the k -th CSTR can be written as follows (Equation (47), see Equations (A76) and (A77) in the Appendix A):

$$\begin{aligned} \frac{V_{R_k}}{F_A^{(0)}} &= \frac{\left(\sum_{h=1}^k S_h \right) x_A^{(k)} - \left(\sum_{h=1}^{k-1} S_h \right) x_A^{(k-1)}}{(-r_A)_k}, \quad \sum_{k=1}^r S_k = 1 \\ \frac{V_{R_k}}{F_A^{(0)}} \Big|_{S_k=S} &= S \frac{[kx_A^{(k)} - (k-1)x_A^{(k-1)}]}{(-r_A)_k}, \quad \sum_{k=1}^r S = rS = 1 \end{aligned} \quad (47)$$

The energy balance on the k -th mixing node is obtained as follows (Equation (48), see Equation (A85) in the Appendix A):

$$\begin{aligned} T_0^{(k)} &= \frac{w_1}{w_1+w_2} T^{(k-1)} + \frac{w_2}{w_1+w_2} T^{(0)} \\ w_1 &\equiv \left[\left(\sum_{h=1}^{k-1} S_h \right) \tilde{C}p_A + \sum_{i=2}^n \theta_i \tilde{C}p_i + \left(\sum_{h=1}^{k-1} S_h \right) \Delta \tilde{C}p_A x_A^{(k-1)} \right] \\ w_2 &\equiv S_k \tilde{C}p_A \end{aligned} \quad (48)$$

If $\sim \tilde{C}p_A$ is negligible, we obtain Equation (49) (see Equation (A86) in the Appendix A):

$$\begin{aligned} T_0^{(k)} &\cong \frac{w_1}{w_1+w_2} T^{(k-1)} + \frac{w_2}{w_1+w_2} T^{(0)} \\ w_1 &\equiv \left[\left(\sum_{h=1}^{k-1} S_h \right) \tilde{C}p_A + \sum_{i=2}^n \theta_i \tilde{C}p_i \right] \\ w_2 &\equiv S_k \tilde{C}p_A \end{aligned} \quad (49)$$

For equal split ratios, we obtain the following expression (Equation (A50), see Equation (A87) in the Appendix A):

$$T_0^{(k)} \Big|_{S_k=S} = \frac{\left[(k-1) S \tilde{C}p_A + \sum_{i=2}^n \theta_i \tilde{C}p_i \right] T^{(k-1)} + S \tilde{C}p_A T^{(0)}}{\left[(k-1) S \tilde{C}p_A + \sum_{i=2}^n \theta_i \tilde{C}p_i + S \tilde{C}p_A \right]} \quad (50)$$

The energy balance on the k -th PFR is obtained as follows (Equation (51), see Equation (A92) in the Appendix A):

$$\begin{aligned} &\left[\begin{array}{c} \text{Thermal contribution of the feed} \\ \left(\tilde{C}p_S - \tilde{C}p_A \right) \\ \text{Contribution of the species other than A} \end{array} + \begin{array}{c} \left(\sum_{h=1}^k S_h \right) \tilde{C}p_A \\ \text{Contribution of the species A} \end{array} + \begin{array}{c} \text{Non-linear contribution} \\ \left(\sum_{h=1}^k S_h \right) x_A \Delta \tilde{C}p_A \end{array} \right] \frac{dT}{dV} = \begin{array}{c} \text{Reaction Contribution} \\ \left(\sum_{h=1}^k S_h \right) \left[-\Delta \tilde{H}_{r,A} \right] \left[\frac{dx_A}{dV} \right] \end{array} \\ \text{Standalone PFR : } &\left(\begin{array}{cc} \text{Thermal contribution of the feed} & \text{Non-linear contribution} \\ \tilde{C}p_S & + \quad x_A \Delta \tilde{C}p_A \end{array} \right) \frac{dT}{dV} = \begin{array}{c} \text{Reaction Contribution} \\ \left[-\Delta \tilde{H}_{r,A} \right] \frac{dx_A}{dV} \end{array} \end{aligned} \quad (51)$$

In particular, in Equation (51), the energy balance of the standalone PFR is also reported for comparison in order to highlight analogies and differences. As for the analogies, the structure of the equations is similar, with the presence of terms identifying the thermal contribution of the feed, the non-linear contribution, and the reaction contribution to the overall thermic extent of the system.

As for the differences, analysing the thermal contribution of the feed, it is clear the split of this contribution into two parts, respectively related to (1) the reactants fed in an all-in-one mode and (2) the part of the key-species (A) that is fed in a distributed way along

the reactors series up to the k -th reactor. That is the reason why the overall contribution of species A is lower than in the standalone case.

We can make an analogous consideration for the non-linear contribution and for the reaction contribution, which are both lowered by the fraction of species A fed up to that reactor.

As for the energy balance on the k -th CSTR of the series, it is obtained as follows (Equation (52), see Equation (A96) in the Appendix A):

$$\left[(\tilde{C}p_s - \tilde{C}p_A) + \left(\sum_{h=1}^k S_h \right) \tilde{C}p_A \right] (T_0^{(k)} - T^{(k)}) + \left(\sum_{h=1}^k S_h \right) [x_{A,0}^{(k)} \Delta \tilde{H}_{r,A}(T_0^{(k)}) - x_A^{(k)} \Delta \tilde{H}_{r,A}(T^{(k)})] = 0 \quad (52)$$

If the enthalpy of reaction can be considered constant, the previous expression is simplified as follows (Equation (53), see Equation (A100) in the Appendix A):

$$\begin{aligned} & \left(\sum_{h=1}^k S_h \right) [x_A^{(k)} - x_A^{(k-1)}] + S_k \left[x_A^{(k-1)} - \underbrace{x_A^{(0)}}_{=0} \right] \\ &= \frac{\left(\sum_{h=1}^k S_h \right) \tilde{C}p_A + (\tilde{C}p_s - \tilde{C}p_A)}{(-\Delta \tilde{H}_{r,A})} (T^{(k)} - T^{(k-1)}) \\ &+ \frac{S_k \tilde{C}p_A}{(-\Delta \tilde{H}_{r,A})} (T^{(k-1)} - T^{(0)}) \end{aligned} \quad (53)$$

where it is also reported as the initial (null) conversion to highlight the analogy between conversion and temperature differences.

Figure 12 shows a numerical example of the calculation of the intermediate inlet conversions of the three reactors in the scheme. As input data, we consider certain values of conversions at the reactor's outlet and the split ratios as known, calculating the corresponding missing conversion data from setting and solving the mass balances at the mixing nodes written in terms of conversion.

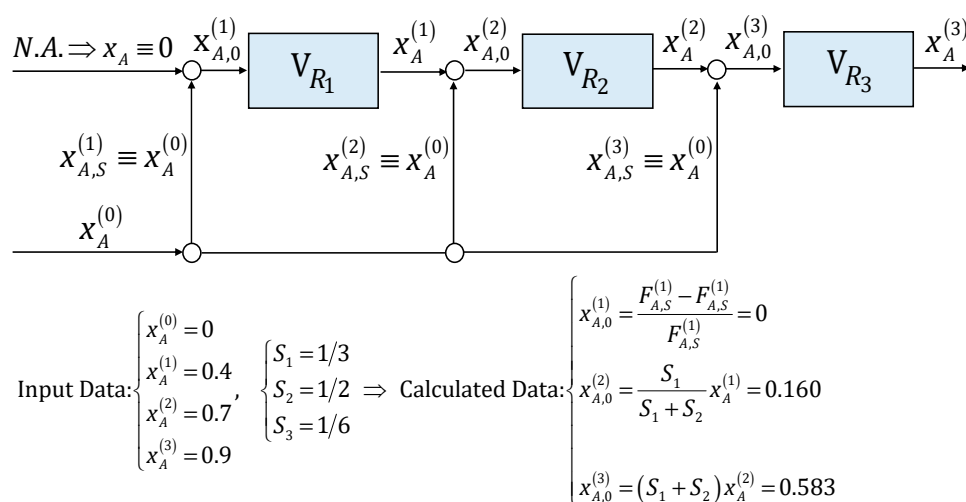


Figure 12. Example of application of the presented approach in terms of calculation of inlet conversions to reactors.

Overall, we highlight that, for an infinite number of infinitesimal reactors—composed of either PFRs or CSTRs—this system in fact coincides with a reactor that in the literature is referred to as *Differential Sidestream Reactors* (DSR) [3], which is of practical importance in a number of applications of interest, especially in the pharmaceutical industry.

4. Conclusions

In this work, a novel systematic way to obtain the design equations (heat and mass balances) of networks of ideal reactors (PFRs and CSTRs) was presented. For this purpose, a general definition of reaction degree and conversion was provided, considering, after validation with well-known reactor systems, several case studies of real systems of interest in chemical engineering as examples of application: (a) adiabatic-stage split reactors, (b) adiabatic-stage reactors intercooled by reactants and (c) adiabatic-stage reactors with interstage distributed feed. The methodology illustrated in this work also allows one to combine different types of reactors in the same network, widening the generality of the presented approach.

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Data Availability Statement: Data are contained within the article.

Conflicts of Interest: The author declares no conflict of interest.

Abbreviations

$\tilde{C}_p$	Specific heat, J mol ⁻¹ K ⁻¹
F	Flow rate, mol s ⁻¹
H	Molar enthalpy, J mol ⁻¹ K ⁻¹
$\{n, m, r, b\}$	Number of: {species, reactions, reactors, network branches}
r_A	Reaction rate (of the key-species A), mol s ⁻¹ m ⁻³
R_k	Recycle ratio (at the k -th reactors)
S_k	Split ratio (at the k -th reactors)
T	Temperature, K
V	Volume, m ³
x_A	Conversion (of the key-species)

Greek Symbols

θ_i	Feed ratio, mol _i mol _A ⁻¹
ν_{ij}	Stoichiometric coefficients
ξ_j	Reaction extent for the j th reaction

Subscripts/Superscripts

f	Final (with respect to a stage with recycle or split)
$\{i, j, k, l\}$	Indices for: {species, reactions, reactors, network branches}
r	Reaction (enthalpy of) or number of reactors
r, A	Reaction enthalpy expressed per mole of A consumed
ref	Reference (temperature)
S	Summation (referred to specific heat)
$*$	Refers to the network in the absence of a reaction
0	Reference state (enthalpy)
IG	Ideal gas
Res	Residual quantity (with respect to the ideal-gas state)

Appendix A. Detailed Development of Design Equations

Appendix A.1. Enthalpy and Flow Rate Expressions

In general, the enthalpy rate of the i -th species in the l -th branch of the network can be written in molar form as follows (Equation (A1)):

$$F_i^{(l)} \tilde{H}_i^{(l)} = \left\{ \begin{array}{l} \text{Enthalpy Rate of} \\ i\text{-th Species on} \\ \text{the } l\text{-th Branch} \end{array} \right\} \quad (\text{A1})$$

By neglecting any possible mixing enthalpy, which is usually negligible in chemical reactors, the enthalpy rate of the i -th species can be expressed as a function of pressure and temperature as (Equation (A2)):

$$\tilde{H}_i(T, P) = \left\{ \begin{array}{l} \tilde{H}_i^{IG}(T), \text{ Ideal Gas} \\ \tilde{H}_i^{IG}(T) + \Delta \tilde{H}_i^{Res}(T, P), \text{ Real Gas} \\ \tilde{H}_i^L(T), \text{ Liquid} \end{array} \right. \quad (\text{A2})$$

$$\begin{aligned} \tilde{H}_i^{IG}(T) &= \Delta \tilde{H}_{f,i}^{IG}(T_{ref}) + \tilde{C}p_i^{IG}(T - T_{ref}) \equiv \Delta \tilde{H}_i^{0,IG} + \tilde{C}p_i^{IG}(T - T_{ref}) \\ \tilde{H}_i^L(T) &= \Delta \tilde{H}_{f,i}^L(T_{ref}) + \tilde{C}p_i^L(T - T_{ref}) \equiv \Delta \tilde{H}_i^{0,L} + \tilde{C}p_i^L(T - T_{ref}) \\ \Delta \tilde{H}_i^{Res}(T, P) &\Leftarrow \text{Equation of State for Real Gases} \end{aligned}$$

where we suppose that all specific heats are constant with temperature within the temperature range considered. Should such a hypothesis become too strong—and this occurs typically for highly exothermic/endothermic reactions in the gas phase—we would need to evaluate the integral of specific heats using, for example, temperature-dependent polynomial forms.

Provided that, neglecting also the non-ideal contribution for the real gases (which anyway is usually small unless working at relatively high pressure), the enthalpy of the i -th species in the l -th branch of the network can be expressed as (Equation (A3)):

$$\tilde{H}_i^{(l)} = \left[\Delta \tilde{H}_{f,i}^0 + \tilde{C}p_i(T^{(l)} - T_{ref}) \right] \quad (\text{A3})$$

where $\Delta \tilde{H}_{f,i}^0$ and T_{ref} are the standard enthalpy of formation and the corresponding reference temperature (usually 298.15 K), respectively.

According to the extended definition of conversion reported in Equations (1) and (2), the flow rate of the i -th species is expressed in terms of conversion as follows (Equation (A4)):

$$F_i^{(l)} = F_A^{*(l)} \left(\theta_i + \frac{\nu_i}{a} x_A^{(l)} \right) \quad (\text{A4})$$

where $F_A^{*(l)}$ is the flow rate of the limiting reactant (i.e., the key-species) in the l -th branch of the network in the absence of a reaction. Therefore, combining the previous expressions, we obtain Equation (A5):

$$F_i^{(l)} \tilde{H}_i^{(l)} = F_A^{*(l)} \left(\theta_i + \frac{\nu_i}{a} x_A^{(l)} \right) \left[\Delta \tilde{H}_i^0 + \tilde{C}p_i(T - T_{ref}) \right] \quad (\text{A5})$$

Equation (A5) is the expression of the enthalpy rate that will be used to obtain the design equations for all the cases considered in this work, given that it can also be used to develop the design equations for other systems.

Appendix A.2. Adiabatic-Stage Reactors with Recycle

Appendix A.2.1. Mass Balances

Mass Balance on the Mixing Nodes

The flow rates in the k -th branch of the reactor network can be expressed as functions of the conversion and of the respective no-reaction flow rates in that branch (Equation (A6)):

$$\begin{aligned} F_{A,0}^{(k)} &= F_{A,0}^{*(k)} (1 - x_{A,0}^{(k)}) = (R_k + 1) F_{A,f}^{(0)} (1 - x_{A,0}^{(k)}) \\ F_A^{(k)} &= F_A^{*(k)} (1 - x_A^{(k)}) = (R_k + 1) F_{A,f}^{(0)} (1 - x_A^{(k)}) \end{aligned} \quad (\text{A6})$$

To obtain the design equations in canonical form, beside the mass and energy balances on the reactors, it is also necessary to make balances on the mixing node. This holds not only for this type of reactor network but also for other ones, some of which are reported in the present work. Specifically for this case, the mass balance in the mixing node can be expressed as follows (Equation (A7)):

$$\begin{aligned} F_{A,f}^{(k-1)} + R_k F_{A,f}^{(k)} &= F_{A,0}^{(k)} \\ F_{A,f}^{(0)} (1 - x_{A,f}^{(k-1)}) + R_k F_{A,f}^{(0)} (1 - x_{A,f}^{(k)}) &= (R_k + 1) F_{A,f}^{(0)} (1 - x_{A,0}^{(k)}) \end{aligned} \quad (\text{A7})$$

Equation (A7) leads to expressing the conversion at the reactor inlet as a function of the conversion at the reactor outlet, which coincides with that at the outlet of the stage (Equation (A8)):

$$x_{A,0}^{(k)} = \frac{1}{(R_k + 1)} x_{A,f}^{(k-1)} + \frac{R_k}{(R_k + 1)} x_{A,f}^{(k)} \quad (\text{A8})$$

It is useful to show that, if we write Equation (A7) for a generic species of the stream (reported in Equation (A9)), we obtain the same expression as that reported in Equation (A8):

$$\begin{aligned} F_{i,f}^{(k-1)} + R_k F_{i,f}^{(k)} &= F_{i,0}^{(k)} \\ \begin{cases} F_{i,f}^{(k-1)} = F_{A,f}^{*(k-1)} \left(\theta_i + \frac{v_i}{a} x_{A,f}^{(k-1)} \right) = F_{A,f}^{(0)} \left(\theta_i + \frac{v_i}{a} x_{A,f}^{(k-1)} \right) \\ F_{i,f}^{(k)} = F_{A,f}^{*(k)} \left(\theta_i + \frac{v_i}{a} x_{A,f}^{(k)} \right) = F_{A,f}^{(0)} \left(\theta_i + \frac{v_i}{a} x_{A,f}^{(k)} \right) \\ F_{i,0}^{(k)} = F_{A,0}^{*(k)} \left(\theta_i + \frac{v_i}{a} x_{A,0}^{(k)} \right) = (R_k + 1) F_{A,f}^{(0)} \left(\theta_i + \frac{v_i}{a} x_{A,f}^{(k-1)} \right) \end{cases} \\ \Downarrow \\ F_{A,f}^{(0)} \left(\theta_i + \frac{v_i}{a} x_{A,f}^{(k-1)} \right) + R_k F_{A,f}^{(0)} \left(\theta_i + \frac{v_i}{a} x_{A,f}^{(k)} \right) &= (R_k + 1) F_{A,f}^{(0)} \left(\theta_i + \frac{v_i}{a} x_{A,0}^{(k)} \right) \\ \left(\theta_i + \frac{v_i}{a} x_{A,f}^{(k-1)} \right) + \left(\theta_i + \frac{v_i}{a} x_{A,f}^{(k)} \right) &= (R_k + 1) \left(\theta_i + \frac{v_i}{a} x_{A,0}^{(k)} \right) \\ \Downarrow \\ x_{A,0}^{(k)} &= \frac{1}{(R_k + 1)} x_{A,f}^{(k-1)} + \frac{R_k}{(R_k + 1)} x_{A,f}^{(k)} \end{aligned} \quad (\text{A9})$$

This occurrence indicates once more the self-consistency of the so-extended definition of conversion.

Mass Balance on PFR

The general design equation for the generic k -th PFR, expressed in terms of the key-species A, mostly taken as the limiting reactant, is (Equation (A10)):

$$\frac{dF_A}{dV} = r_A \quad (\text{A10})$$

which can be expressed in terms of conversion as follows (Equations (A11)):

$$\begin{aligned} (R_k + 1)F_{A,f}^{(0)} \frac{dx_A}{dV} &= (-r_A) \\ (R_k + 1) \int_{x_{A,0}^{(k)}}^{x_A^{(k)}} \frac{dx_A}{(-r_A)} &= \frac{V_{R_k}}{F_{A,f}^{(0)}} \end{aligned} \quad (\text{A11})$$

The final expression of the *PFR* design equation, obtained by replacing the inlet “local” conversions $x_{A,0}^{(k)}$ and $x_A^{(k)}$ with its expression in terms of stage conversions $x_{A,f}^{(k-1)}$ and $x_{A,f}^{(k)}$, is (Equation (A12)):

$$\frac{V_{R_k}}{F_{A,f}^{(0)}} = (R_k + 1) \int_{\frac{1}{(R_k+1)}x_{A,f}^{(k-1)} + \frac{R_k}{(R_k+1)}x_{A,f}^{(k)}}^{x_{A,f}^{(k)}} \frac{dx_A}{(-r_A)} \quad (\text{A12})$$

Mass Balance on CSTR

As for *CSTR*, the mass balance can be written as follows (Equation (A13)):

$$F_{A,0}^{(k)} - F_A^{(k)} + r_{A_k} V_{R_k} = 0 \quad (\text{A13})$$

In terms of conversion, we have the following (Equations (A33) and (A34)):

$$(R_k + 1)F_{A,f}^{(0)}(1 - x_{A,0}^{(k)}) - (R_k + 1)F_{A,f}^{(0)}(1 - x_A^{(k)}) + r_{A_k} V_{R_k} = 0 \quad (\text{A14})$$

$$\begin{aligned} \frac{V_{R_k}}{F_{A,f}^{(0)}} &= (R_k + 1) \frac{(x_A^{(k)} - x_{A,0}^{(k)})}{(-r_{A_k})} \\ \frac{V_{R_k}}{F_{A,f}^{(0)}} &= \frac{(x_{A,f}^{(k)} - x_{A,f}^{(k-1)})}{(-r_{A_k})} \end{aligned} \quad (\text{A15})$$

Appendix A.2.2. Energy Balances

Energy Balance on the Mixing Nodes

The energy balance on the mixing nodes of the generic k -th stage is stated in Equation (A16):

$$\begin{aligned} \sum_{i=1}^n F_{i,f}^{(k-1)} \tilde{H}_i(T_f^{(k-1)}) + \sum_{i=1}^n F_{i,R}^{(k)} \tilde{H}_i(T_R^{(k)}) &= \sum_{i=1}^n F_{i,0}^{(k)} \tilde{H}_i(T_0^{(k)}) \\ F_{A,f}^{(0)} \left(\theta_i + \frac{v_i}{a} x_{A,f}^{(k-1)} \right) + R_k F_{A,f}^{(0)} \left(\theta_i + \frac{v_i}{a} x_{A,f}^{(k)} \right) &= (R_k + 1) F_{A,f}^{(0)} \left(\theta_i + \frac{v_i}{a} x_{A,0}^{(k)} \right) \\ F_{A,f}^{(0)} \sum_{i=1}^n \left(\theta_i + \frac{v_i}{a} x_{A,f}^{(k-1)} \right) \left[\Delta \tilde{H}_i^0 + \tilde{C} p_i (T_f^{(k-1)} - T_{ref}) \right] &+ R_k F_{A,f}^{(0)} \sum_{i=1}^n \left(\theta_i + \frac{v_i}{a} x_{A,f}^{(k)} \right) \left[\Delta \tilde{H}_i^0 + \tilde{C} p_i (T_R^{(k)} - T_{ref}) \right] \\ &= (R_k + 1) F_{A,f}^{(0)} \sum_{i=1}^n \left(\theta_i + \frac{v_i}{a} x_{A,0}^{(k)} \right) \left[\Delta \tilde{H}_i^0 + \tilde{C} p_i (T_0^{(k)} - T_{ref}) \right] \\ \tilde{C} p_S T_f^{(k-1)} + x_{A,f}^{(k-1)} \left[\Delta \tilde{H}_{r,A}^0 + \Delta \tilde{C} p_A (T_f^{(k-1)} - T_{ref}) \right] &+ R_k \left[\tilde{C} p_S T_R^{(k)} + x_{A,f}^{(k)} \left[\Delta \tilde{H}_{r,A}^0 + \Delta \tilde{C} p_A (T_R^{(k)} - T_{ref}) \right] \right] \\ &= (R_k + 1) \left[\tilde{C} p_S T_0^{(k)} + x_{A,0}^{(k)} \left[\Delta \tilde{H}_{r,A}^0 + \Delta \tilde{C} p_A (T_0^{(k)} - T_{ref}) \right] \right] \end{aligned} \quad (\text{A16})$$

Inserting Equation (A8) into the last of Equation (A16), the exiting temperature $T_0^{(k)}$ finally results in a weighted average of the temperatures of the entering streams (Equation (A17)):

$$\begin{aligned} T_0^{(k)} &= \frac{1}{(R_k+1)} \left(\frac{\tilde{C}p_S + \Delta\tilde{C}p_A x_{A,f}^{(k-1)}}{\tilde{C}p_S + \Delta\tilde{C}p_A x_{A,0}^{(k)}} \right) T_f^{(k-1)} + \frac{R_k}{(R_k+1)} \left(\frac{\tilde{C}p_S + \Delta\tilde{C}p_A x_{A,f}^{(k)}}{\tilde{C}p_S + \Delta\tilde{C}p_A x_{A,0}^{(k)}} \right) T_f^{(k)} \\ T^{(k)} &= T_f^{(k)} \end{aligned} \quad (\text{A17})$$

In the particular case in which $\Delta\tilde{C}p_A$ can be neglected with respect to $\tilde{C}p_S$ (conversion is always lower than unity), Equation (A17) is simplified as follows (Equation (A18)):

$$T_0^{(k)} = \frac{1}{(R_k+1)} T_f^{(k-1)} + \frac{R_k}{(R_k+1)} T_f^{(k)} \quad (\text{A18})$$

which have the same form as the previously obtained one for conversion (Equation (A8)). This confirms that in a $\{x_A \text{ vs. } T\}$ plot, the working points of the three streams of a mixing node are connected by a straight line.

Energy Balance on PFR

The energy balance for a PFR is expressed as follows (Equation (A19)):

$$\frac{d}{dV} \left(\sum_{i=1}^n F_i \tilde{H}_i \right) = 0 \quad (\text{A19})$$

which leads to Equation (A20) if expressing it in terms of conversion:

$$\begin{aligned} \frac{d}{dV} \left(\sum_{i=1}^n \left[(R_k+1) F_{A,f}^{(0)} \left(\theta_i + \frac{v_i}{a} x_A \right) \right] \left[\Delta\tilde{H}_i^0 + \tilde{C}p_i (T - T_{ref}) \right] \right) &= 0 \\ \frac{d}{dV} \left(\sum_{i=1}^n \left(\theta_i + \frac{v_i}{a} x_A \right) \left[\Delta\tilde{H}_i^0 + \tilde{C}p_i (T - T_{ref}) \right] \right) &= 0 \\ \frac{d}{dV} \left(\left[\tilde{C}p_S (T - T_{ref}) + \Delta\tilde{H}_{r,A}^0 x_A + \Delta\tilde{C}p_A x_A (T - T_{ref}) \right] \right) &= 0 \\ \left(\tilde{C}p_S + \Delta\tilde{C}p_A x_A \right) \frac{dT}{dV} &= \left(-\Delta\tilde{H}_{r,A} \right) \frac{dx_A}{dV} \\ \frac{dT}{dV} &= \frac{(-\Delta\tilde{H}_{r,A}) \frac{dx_A}{dV}}{(\tilde{C}p_S + \Delta\tilde{C}p_A x_A)} \end{aligned} \quad (\text{A20})$$

Inserting the mass balance (Equations (A11)) into Equation (A20), we finally obtain a canonical form of the energy balance for an adiabatic PFR (Equation (A21)).

$$\frac{dT}{dV} = \frac{(-\Delta\tilde{H}_{r,A})(-r_A)}{F_{A,f}^{(0)}(R_k+1) \left(\tilde{C}p_S + \frac{\Delta\tilde{C}p}{a} x_A \right)} \quad (\text{A21})$$

Energy Balance on CSTR

The energy balance for a CSTR can be written as follows (Equation (A22)):

$$\sum_{i=1}^n F_i \tilde{H}_i \Big|_{IN} - \sum_{i=1}^n F_i \tilde{H}_i \Big|_{OUT} = 0 \quad (\text{A22})$$

which leads to Equation (A23):

$$\begin{aligned}
& \sum_{i=1}^n \left[F_{A,f}^{(0)}(R_k + 1) \left(\theta_i + \frac{\nu_i}{a} x_{A,0}^{(k)} \right) \tilde{H}_i(T_0^{(k)}) \right] - \sum_{i=1}^n \left[F_{A,f}^{(0)}(R_k + 1) \left(\theta_i + \frac{\nu_i}{a} x_A^{(k)} \right) \tilde{H}_i(T^{(k)}) \right] = 0 \\
& \sum_{i=1}^n \left[\left(\theta_i + \frac{\nu_i}{a} x_{A,0}^{(k)} \right) \tilde{H}_i(T_0^{(k)}) \right] - \sum_{i=1}^n \left[\left(\theta_i + \frac{\nu_i}{a} x_A^{(k)} \right) \tilde{H}_i(T^{(k)}) \right] = 0 \\
& \sum_{i=1}^n \left(\theta_i + \frac{\nu_i}{a} x_{A,0}^{(k)} \right) \left[\Delta \tilde{H}_i^0(T_{ref}) + \tilde{C}_{p,i}(T_0^{(k)} - T_{ref}) \right] - \sum_{i=1}^n \left(\theta_i + \frac{\nu_i}{a} x_A^{(k)} \right) \left[\Delta \tilde{H}_i^0(T_{ref}) + \tilde{C}_{p,i}(T^{(k)} - T_{ref}) \right] = 0
\end{aligned} \tag{A23}$$

Simplifying appropriately the previous expressions, we obtain (Equation (A24)):

$$\begin{aligned}
& \tilde{C}_{p,S}(T_0^{(k)} - T^{(k)}) + \left[x_{A,0}^{(k)} \Delta \tilde{H}_{r,A}(T_0^{(k)}) - x_A^{(k)} \Delta \tilde{H}_{r,A}(T^{(k)}) \right] = 0 \\
& x_{A,0}^{(k)} = \frac{1}{(R_k + 1)} x_{A,f}^{(k-1)} + \frac{R_k}{(R_k + 1)} x_{A,f}^{(k)}, x_A^{(k)} = x_{A,f}^{(k)}
\end{aligned} \tag{A24}$$

If the reaction enthalpy can be considered the same at inlet and outlet, Equation (A24) assumes the following form in terms of stage conversions (Equation (A25)):

$$\begin{aligned}
& \tilde{C}_{p,S}(T_0^{(k)} - T^{(k)}) + \frac{(-\Delta \tilde{H}_{r,A})}{(R_k + 1)} (x_{A,f}^{(k)} - x_{A,f}^{(k-1)}) = 0 \\
& (x_{A,f}^{(k)} - x_{A,f}^{(k-1)}) = (R_k + 1) \frac{\tilde{C}_{p,S}(T^{(k)} - T_0^{(k)})}{(-\Delta \tilde{H}_{r,A})}
\end{aligned} \tag{A25}$$

Appendix A.3. Adiabatic-Stage Reactors with Split

Appendix A.3.1. Mass Balances

Mass Balance on the Mixing Nodes

The flow rates along the branches of the k -th stage of the series are expressed in terms of conversion as follows (Equation (A26)):

$$\begin{aligned}
F_{A,0}^{(k)} &= F_{A,0}^{*(k)} (1 - x_{A,0}^{(k)}) = (1 - S_k) F_A^{(0)} (1 - x_{A,0}^{(k)}) \\
F_{A,S}^{(k)} &= F_{A,S}^{*(k)} (1 - x_{A,S}^{(k)}) = S_k F_{A,f}^{(0)} (1 - x_{A,S}^{(k)}) \\
F_A^{(k)} &= F_A^{*(k)} (1 - x_A^{(k)}) = (1 - S_k) F_{A,f}^{(0)} (1 - x_A^{(k)})
\end{aligned} \tag{A26}$$

where the split ratios S_k are generally different from each other.

The mass balance on the mixing nodes just after the outlet of each reactor is needed to express the conversion at the outlet of the k -th reactor as a function of the conversions at the inlet and outlet of the stage. Equation (A27) reports the steps from the mass balance to the final expression of the outlet conversion $x_{A,0}$:

$$\begin{aligned}
F_A^{(k)} + S_k F_{A,f}^{(k-1)} &= F_{A,f}^{(k)} \\
(1 - S_k) F_{A,f}^{(0)} (1 - x_A^{(k)}) + S_k F_{A,f}^{(0)} (1 - x_{A,S}^{(k)}) &= F_{A,f}^{(0)} (1 - x_{A,f}^{(k)}) \\
x_A^{(k)} - S_k x_A^{(k)} + S_k x_{A,f}^{(k-1)} &= x_{A,f}^{(k)}
\end{aligned} \tag{A27}$$

which leads to the following final expression (Equation (A28)):

$$x_A^{(k)} = \frac{1}{1 - S_k} x_{A,f}^{(k)} - \frac{S_k}{1 - S_k} x_{A,f}^{(k-1)} \tag{A28}$$

Mass Balance on PFR

We start again from the generic k -th PFR, expressed in terms of the limiting reactant A (Equation (A29)):

$$\frac{dF_A}{dV} = r_A \tag{A29}$$

which can be expressed in terms of conversion as follows (Equation (A30)):

$$(1 - S_k)F_{A,f}^{(0)} \frac{dx_A}{dV} = (-r_A)$$

$$(1 - S_k) \int_{x_{A,0}^{(k)}}^{x_A^{(k)}} \frac{dx_A}{(-r_A)} = \frac{V_{R_k}}{F_{A,f}^{(0)}} \quad (\text{A30})$$

The final expression of the PFR design equation, obtained by replacing the inlet conversion with its expression in terms of stage conversions, is (Equation (A31)):

$$\frac{V_{R_k}}{F_{A,f}^{(0)}} = (1 - S_k) \int_{x_{A,f}^{(k-1)}}^{\frac{1}{1-S_k}x_{A,f}^{(k)} - \frac{S_k}{1-S_k}x_{A,0}^{(k-1)}} \frac{dx_A}{(-r_A)} \quad (\text{A31})$$

Mass Balance on CSTR

As for CSTR, the mass balance can be written as follows (Equation (A32)):

$$F_{A,0}^{(k)} - F_A^{(k)} + r_{A_k} V_{R_k} = 0 \quad (\text{A32})$$

In terms of conversion, we have the following (Equations (A33) and (34)):

$$(1 - S_k)F_{A,f}^{(0)}(1 - x_{A,0}^{(k)}) - (1 - S_k)F_{A,f}^{(0)}(1 - x_A^{(k)}) + r_{A_k} V_{R_k} = 0 \quad (\text{A33})$$

$$\frac{V_{R_k}}{F_{A,f}^{(0)}} = (1 - S_k) \frac{(x_A^{(k)} - x_{A,0}^{(k)})}{(-r_{A_k})}$$

$$\frac{V_{R_k}}{F_{A,f}^{(0)}} = \frac{(x_{A,f}^{(k)} - x_{A,f}^{(k-1)})}{(-r_{A_k})} \quad (\text{A34})$$

Appendix A.3.2. Energy Balances

Energy Balance on the Mixing Nodes

The energy balance on the mixing nodes can be expressed as follows (Equation (A35)):

$$\sum_{i=1}^n F_i^{(k)} \tilde{H}_i(T^{(k)}) + \sum_{i=1}^n F_{i,S}^{(k)} \tilde{H}_i(T_f^{(k-1)}) = \sum_{i=1}^n F_{i,f}^{(k)} \tilde{H}_i(T_f^{(k)})$$

$$\sum_{i=1}^n F_i^{(k)} \tilde{H}_i(T^{(k)}) + \sum_{i=1}^n S_k F_{i,f}^{(k-1)} \tilde{H}_i(T_f^{(k-1)}) = \sum_{i=1}^n F_{i,f}^{(k)} \tilde{H}_i(T_f^{(k)})$$

$$\sum_{i=1}^n (1 - S_k) F_{A,f}^{(0)} \left(\theta_i + \frac{v_i}{a} x_A^{(k)} \right) \left[\Delta \tilde{H}_i^0 + \tilde{C} p_i (T^{(k)} - T_{Ref}) \right]$$

$$+ \sum_{i=1}^n S_k F_{A,f}^{(0)} \left(\theta_i + \frac{v_i}{a} x_{A,f}^{(k-1)} \right) \left[\Delta \tilde{H}_i^0 + \tilde{C} p_i (T_f^{(k-1)} - T_{Ref}) \right]$$

$$= \sum_{i=1}^n F_{A,f}^{(0)} \left(\theta_i + \frac{v_i}{a} x_{A,f}^{(k)} \right) \left[\Delta \tilde{H}_i^0 + \tilde{C} p_i (T_f^{(k)} - T_{Ref}) \right] \quad (\text{A35})$$

$$(1 - S_k) \left[\tilde{C} p_S T^{(k)} + x_A^{(k)} \Delta \tilde{H}_{r,A}(T_k) \right]$$

$$+ S_k \left[\tilde{C} p_S T_f^{(k-1)} + x_{A,f}^{(k-1)} \Delta \tilde{H}_{r,A}(T_f^{(k-1)}) \right]$$

$$= \left[\tilde{C} p_S T_f^{(k)} + x_{A,f}^{(k)} \Delta \tilde{H}_{r,A}(T_f^{(k)}) \right]$$

which leads to the following explicit expression (Equation (A36)):

$$T^{(k)} = \frac{\left(\tilde{C}p_S + \Delta\tilde{C}p_A x_{A,f}^{(k)}\right) T_f^{(k)} - S_k \left(\tilde{C}p_S + \Delta\tilde{C}p_A x_{A,f}^{(k-1)}\right) T_f^{(k-1)}}{\left[\left(\tilde{C}p_S + \Delta\tilde{C}p_A x_{A,f}^{(k)}\right) - S_k \left(\tilde{C}p_S + \Delta\tilde{C}p_A x_{A,f}^{(k-1)}\right)\right]} \quad (\text{A36})$$

If $\Delta\tilde{C}p_A$ can be neglected with respect to $\tilde{C}p_S$, Equation (A36) can be simplified as follows (Equation (A37)):

$$T^{(k)} = \frac{1}{(1 - S_k)} T_f^{(k)} - \frac{S_k}{(1 - S_k)} T_f^{(k-1)} \quad (\text{A37})$$

Energy Balance on PFR

The energy balance on the generic k -th PFR is written as follows (Equation (A38)):

$$\begin{aligned} \frac{d}{dV} \left(\sum_{i=1}^n \left[(1 - S_k) F_{A,f}^{(0)} \left(\theta_i + \frac{v_i}{a} x_A \right) \right] \left[\Delta\tilde{H}_i^0 + \tilde{C}p_i (T - T_{ref}) \right] \right) &= 0 \\ \left(\tilde{C}p_S + \Delta\tilde{C}p_A x_A \right) \frac{dT}{dV} &= \left(-\Delta\tilde{H}_{r,A} \right) \frac{dx_A}{dV} \\ \frac{dT}{dV} &= \frac{(-\Delta\tilde{H}_{r,A}) \frac{dx_A}{dV}}{(\tilde{C}p_S + \Delta\tilde{C}p_A x_A)} \end{aligned} \quad (\text{A38})$$

Combining Equation (A30) (differential mass balance) and Equation (A38), we finally obtain the following expression (Equation (A39)):

$$\frac{dT}{dV} = \frac{\left(-\Delta\tilde{H}_{r,A} \right) (-r_A)}{F_{A,f}^{(0)} (1 - S_k) \left(\tilde{C}p_S + \frac{\Delta\tilde{C}p}{a} x_A \right)} \quad (\text{A39})$$

Energy Balance on CSTR

The general expression of the energy balance on the generic k -th CSTR is (Equation (A40)):

$$\sum_{i=1}^n F_i \tilde{H}_i \Big|_{IN} - \sum_{i=1}^n F_i \tilde{H}_i \Big|_{OUT} = 0 \quad (\text{A40})$$

which leads to Equation (A.41) when expressing the flow rates in terms of the respective conversions:

$$\begin{aligned} \sum_{i=1}^n \left[F_{A,f}^{(0)} (1 - S_k) \left(\theta_i + \frac{v_i}{a} x_{A,0}^{(k)} \right) \tilde{H}_i \left(T_0^{(k)} \right) \right] - \sum_{i=1}^n \left[F_{A,f}^{(0)} (1 - S_k) \left(\theta_i + \frac{v_i}{a} x_A^{(k)} \right) \tilde{H}_i \left(T^{(k)} \right) \right] &= 0 \\ \sum_{i=1}^n \left[\left(\theta_i + \frac{v_i}{a} x_{A,0}^{(k)} \right) \tilde{H}_i \left(T_0^{(k)} \right) \right] - \sum_{i=1}^n \left[\left(\theta_i + \frac{v_i}{a} x_A^{(k)} \right) \tilde{H}_i \left(T^{(k)} \right) \right] &= 0 \end{aligned} \quad (\text{A41})$$

Simplifying appropriately the previous expressions and expressing the outlet conversion as a function of the stage conversions, we obtain (Equation (A42)):

$$\begin{aligned} \tilde{C}p_S \left(T_0^{(k)} - T^{(k)} \right) + \left[x_{A,0}^{(k)} \Delta\tilde{H}_{r,A} \left(T_0^{(k)} \right) - x_A^{(k)} \Delta\tilde{H}_{r,A} \left(T^{(k)} \right) \right] &= 0 \\ x_A^{(k)} = \frac{1}{1 - S_k} x_{A,f}^{(k)} - \frac{S_k}{1 - S_k} x_{A,f}^{(k-1)}, \quad x_{A,0}^{(k)} &= x_{A,f}^{(k-1)} \end{aligned} \quad (\text{A42})$$

If the reaction enthalpy can be considered the same at the inlet and outlet ($\Delta\tilde{C}p_A \approx 0$), Equation (A42) assumes the following form in terms of stage conversions (Equation (A43)):

$$\begin{aligned} \tilde{C}p_S \left(T_0^{(k)} - T^{(k)} \right) + \frac{(-\Delta\tilde{H}_{r,A})}{1 - S_k} \left[x_{A,f}^{(k)} - x_{A,f}^{(k-1)} \right] &= 0 \\ \left(x_{A,f}^{(k)} - x_{A,f}^{(k-1)} \right) &= (1 - S_k) \frac{\tilde{C}p_S \left(T^{(k)} - T_0^{(k)} \right)}{(-\Delta\tilde{H}_{r,A})} \end{aligned} \quad (\text{A43})$$

Expressing inlet and outlet temperatures as functions of the respective stage temperatures, we obtain the following expression (Equation (A44)), in which there is no formal dependency on the split ratio:

$$\begin{aligned} T_0^{(k)} &= T_f^{(k-1)}, T^{(k)} = \frac{1}{(1-S_k)} T_f^{(k)} - \frac{S_k}{(1-S_k)} T_f^{(k-1)} \\ \left(x_{A,f}^{(k)} - x_{A,f}^{(k-1)} \right) &= \frac{\tilde{C}_{pS} (T_f^{(k)} - T_f^{(k-1)})}{(-\Delta \bar{H}_{r,A})} \end{aligned} \quad (\text{A44})$$

Appendix A.4. Adiabatic-Stage Reactors Intercooled/Interheated by Reactants

Appendix A.4.1. Mass Balances

Mass Balance on the Mixing Nodes

Similarly to what was performed in the previous cases, we make here the mass balance on the mixing nodes to express the inlet conversion as a function of the outlet ones (Equation (A45)):

$$\begin{aligned} F_A^{(k-1)} + F_{A,S}^{(k)} &= F_{A,0}^{(k)} \\ F_A^{(k-1)} + S_k F_A^{(0)} &= F_{A,0}^{(k)} \end{aligned} \quad (\text{A45})$$

Such a balance can be serialised to the k -th node, as shown in Equation (A46):

$$\begin{aligned} F_{A,0}^{(1)} &= F_{A,0}^{*(1)} (1 - x_{A,0}^{(1)}) = S_1 F_A^{(0)} (1 - x_{A,0}^{(1)}) = S_1 F_A^{(0)} \\ F_A^{(1)} &= F_A^{*(1)} (1 - x_A^{(1)}) = S_1 F_A^{(0)} (1 - x_A^{(1)}) \\ F_{A,0}^{(2)} &= F_{A,0}^{*(2)} (1 - x_{A,0}^{(2)}) = (S_1 + S_2) F_A^{(0)} (1 - x_{A,0}^{(2)}) \\ F_A^{(2)} &= F_A^{*(2)} (1 - x_A^{(2)}) = (S_1 + S_2) F_A^{(0)} (1 - x_A^{(2)}) \\ &\dots \\ F_{A,0}^{(k)} &= F_{A,0}^{*(k)} (1 - x_{A,0}^{(k)}) = \left(\sum_{h=1}^k S_h \right) F_A^{(0)} (1 - x_{A,0}^{(k)}) \\ F_A^{(k)} &= F_A^{*(k)} (1 - x_A^{(k)}) = \left(\sum_{h=1}^k S_h \right) F_A^{(0)} (1 - x_A^{(k)}) \\ \sum_{h=1}^r S_h &= 1 \end{aligned} \quad (\text{A46})$$

Therefore, we obtain the following compact form stating the relationship among conversions (Equation (A47)):

$$\left(\sum_{h=1}^{k-1} S_h \right) (1 - x_A^{(k-1)}) + S_k = \left(\sum_{h=1}^k S_h \right) (1 - x_{A,0}^{(k)}) \quad (\text{A47})$$

Making the inlet conversion explicit, we obtain (Equation (A48)):

$$\begin{aligned} x_{A,0}^{(k)} &= \frac{\sum_{h=1}^{k-1} S_h}{\sum_{h=1}^k S_h} x_A^{(k-1)} \\ x_{A,0}^{(k)} \Big|_{S_k=S} &= \frac{k-1}{k} x_A^{(k-1)} \end{aligned} \quad (\text{A48})$$

Mass Balance on PFR

The differential form of the mass balance on PFR is (Equation (A49)):

$$\frac{dF_A}{dV} = r_A \Big|_{R_k} \quad (\text{A49})$$

Using the general definition of conversion on the reactor branch, we obtain Equation (A50):

$$\begin{aligned} F_A &= \left(\sum_{h=1}^k S_h \right) F_A^{(0)} (1 - x_A) \\ \left(\sum_{h=1}^k S_h \right) F_A^{(0)} \frac{dx_A}{dV} &= (-r_A)|_{R_k} \end{aligned} \quad (\text{A50})$$

The corresponding integral form is obtained (Equation (A51)):

$$\frac{V_{R_k}}{F_A^{(0)}} = \left(\sum_{h=1}^k S_h \right) \int_{\frac{\sum_{h=1}^{k-1} S_h}{\sum_{h=1}^k S_h} x_A^{(k-1)}}^{x_A^{(k)}} \frac{dx_A}{(-r_A)} \quad (\text{A51})$$

For equal values of split ratio, we can simplify Equation (A51) as follows (Equation (A52)):

$$\frac{V_{R_k}}{F_A^{(0)}} \Big|_{S_k=S} = kS \int_{\frac{k-1}{k} x_A^{(k-1)}}^{x_A^{(k)}} \frac{dx_A}{(-r_A)} \quad (\text{A52})$$

Mass Balance on CSTR

The mass balance on the k -th CSTR is written as follows (Equation (A53)):

$$F_{A,0}^{(k)} - F_A^{(k)} = V_{R_k} (-r_A)|_{R_k} \quad (\text{A53})$$

Expressing the flow rates as functions of the respective conversions, we obtain (Equation (A54)):

$$\begin{aligned} F_A^{(k)} &= \left(\sum_{h=1}^k S_h \right) F_A^{(0)} (1 - x_A^{(k)}) \\ F_{A,0}^{(k)} &= \left(\sum_{h=1}^k S_h \right) F_A^{(0)} (1 - x_{A,0}^{(k)}) \\ \left(\sum_{h=1}^k S_h \right) F_A^{(0)} (1 - x_{A,0}^{(k)}) - \left(\sum_{h=1}^k S_h \right) F_A^{(0)} (1 - x_A^{(k)}) &= V_{R_k} (-r_A)|_{R_k} \\ \frac{V_{R_k}}{F_A^{(0)}} &= \left(\sum_{h=1}^k S_h \right) \frac{(x_A^{(k)} - x_{A,0}^{(k)})}{(-r_A)_k} \end{aligned} \quad (\text{A54})$$

Expressing the inlet conversion as a function of the outlet conversion of the previous stage, we obtain Equation (A55):

$$\begin{aligned} \frac{V_{R_k}}{F_A^{(0)}} &= \frac{\left[\left(\sum_{h=1}^k S_h \right) x_A^{(k)} - \left(\sum_{h=1}^{k-1} S_h \right) x_A^{(k-1)} \right]}{(-r_A)_k} \\ \frac{V_{R_k}}{F_A^{(0)}} \Big|_{S_k=S} &= S \frac{[kx_A^{(k)} - (k-1)x_A^{(k-1)}]}{(-r_A)_k} \end{aligned} \quad (\text{A55})$$

Appendix A.4.2. Energy Balances

Energy Balance on the Mixing Nodes

The energy (enthalpy) balance on the mixing nodes is reported in Equation (A56):

$$\sum_{i=1}^n F_i^{(k-1)} \tilde{H}_i(T^{(k-1)}) + \sum_{i=1}^n F_{i,S}^{(k)} \tilde{H}_i(T^{(0)}) = \sum_{i=1}^n F_{i,0}^{(k)} \tilde{H}_i(T_0^{(k)}) \quad (\text{A56})$$

Expressing Equation (A56) in terms of conversions, Equation (A57) is obtained:

$$\begin{aligned} & \sum_{i=1}^n \left(\sum_{h=1}^{k-1} S_h \right) F_A^{(0)} \left(\theta_i + \frac{\nu_i}{a} x_A^{(k-1)} \right) \tilde{H}_i \left(T^{(k-1)} \right) + \sum_{i=1}^n S_k F_A^{(0)} \theta_i \tilde{H}_i \left(T^{(0)} \right) \\ &= \sum_{i=1}^n \left(\sum_{h=1}^k S_h \right) F_A^{(0)} \left(\theta_i + \frac{\nu_i}{a} x_{A,0}^{(k)} \right) \tilde{H}_i \left(T_0^{(k)} \right) \end{aligned} \quad (\text{A57})$$

Using some algebraic calculations, Equation (A57) is expressed in terms of specific heat and enthalpy of reaction (Equation (A58)):

$$\begin{aligned} & \left[\tilde{C}_p S T^{(k-1)} \left(\sum_{h=1}^{k-1} S_h \right) + x_A^{(k-1)} \left(\sum_{h=1}^{k-1} S_h \right) \Delta \tilde{H}_{r,A} \left(T^{(k-1)} \right) \right] + S_k \tilde{C}_p S T^{(0)} \\ &= \left[\tilde{C}_p S T_0^{(k)} \left(\sum_{h=1}^k S_h \right) + x_{A,0}^{(k)} \left(\sum_{h=1}^k S_h \right) \Delta \tilde{H}_{r,A} \left(T_0^{(k)} \right) \right] \\ & \left[\tilde{C}_p S T^{(k-1)} \left(\sum_{h=1}^{k-1} S_h \right) + x_A^{(k-1)} \left(\sum_{h=1}^{k-1} S_h \right) \left[\Delta \tilde{C}_p A \left(T^{(k-1)} - T_0^{(k)} \right) \right] \right] + S_k \tilde{C}_p S T^{(0)} = \left[\tilde{C}_p S T_0^{(k)} \left(\sum_{h=1}^k S_h \right) \right] \\ & \Delta \tilde{C}_p A \equiv \frac{\Delta \tilde{C}_p}{a} \end{aligned} \quad (\text{A58})$$

Finally, we obtain the inlet temperature as the weighted mean value of the outlet temperature of the previous stage and the initial temperature (Equation (A59)):

$$T_0^{(k)} = \frac{\left(\sum_{h=1}^{k-1} S_h \right) \left[\tilde{C}_p S + x_A^{(k-1)} \Delta \tilde{C}_p A \right]}{\left(\sum_{h=1}^k S_h \right) \left[\tilde{C}_p S + x_{A,0}^{(k)} \Delta \tilde{C}_p A \right]} T^{(k-1)} + \frac{S_k \tilde{C}_p S}{\left(\sum_{h=1}^k S_h \right) \left[\tilde{C}_p S + x_{A,0}^{(k)} \Delta \tilde{C}_p A \right]} T^{(0)} \quad (\text{A59})$$

If $\Delta \tilde{C}_p A \approx 0$, we obtain the following expressions for the inlet temperature (Equation (A60)):

$$\begin{aligned} T_0^{(k)} &= \frac{\left(\sum_{h=1}^{k-1} S_h \right)}{\left(\sum_{h=1}^k S_h \right)} T^{(k-1)} + \frac{S_k}{\left(\sum_{h=1}^k S_h \right)} T^{(0)} \\ T_0^{(k)} \Big|_{S_k=S} &= \frac{k-1}{k} T^{(k-1)} + \frac{1}{k} T^{(0)} \end{aligned} \quad (\text{A60})$$

Energy Balance on PFR

The energy balance on PFR is expressed as follows (Equation (A61)):

$$\begin{aligned} & \frac{d}{dV} \left(\sum_{i=1}^n \left(\sum_{h=1}^k S_h \right) F_A^{(0)} \left(\theta_i + \frac{\nu_i}{a} x_A \right) \left[\Delta \tilde{H}_{f,i}^0 + \tilde{C}_p i \left(T - T_{ref} \right) \right] \right) = 0 \\ & \sum_{i=1}^n \left(\frac{\nu_i}{a} \frac{dx_A}{dV} \right) \left[\Delta \tilde{H}_{f,i}^0 + \tilde{C}_p i \left(T - T_{ref} \right) \right] + \sum_{i=1}^n \left(\theta_i + \frac{\nu_i}{a} x_A \right) \tilde{C}_p i \frac{dT}{dV} = 0 \\ & \frac{dx_A}{dV} \sum_{i=1}^n \left[\frac{\nu_i}{a} \Delta \tilde{H}_{f,i}^0 + \frac{\nu_i}{a} \tilde{C}_p i \left(T - T_{ref} \right) \right] + \frac{dT}{dV} \sum_{i=1}^n \left(\theta_i \tilde{C}_p i + \frac{\nu_i}{a} \tilde{C}_p i x_A \right) = 0 \\ & \Delta \tilde{H}_{r,A} \frac{dx_A}{dV} + \left(\tilde{C}_p S + \Delta \tilde{C}_p A x_A \right) \frac{dT}{dV} = 0 \\ & \left(\tilde{C}_p S + \Delta \tilde{C}_p A x_A \right) \frac{dT}{dV} = \left(-\Delta \tilde{H}_{r,A} \right) \frac{dx_A}{dV} \end{aligned} \quad (\text{A61})$$

After substituting the expression of the conversion derivative in terms of reaction rate, the differential equation reported in Equation (A62) is obtained:

$$\begin{cases} \frac{dT}{dV} = \frac{(-\Delta\tilde{H}_{r,A})(-r_A)}{\left(\sum_{h=1}^k S_h\right)F_A^{(0)}(\tilde{C}p_S + \Delta\tilde{C}p_A x_A)} \\ T(V_k = 0) = T_0^{(k)} \end{cases} \quad (\text{A62})$$

If the split ratios are equal, Equation (A62) turns into Equation (A63):

$$\begin{cases} \left.\frac{dT}{dV}\right|_{S_k=S} = \frac{(-\Delta\tilde{H}_{r,A})(-r_A)}{kS F_A^{(0)}(\tilde{C}p_S + \Delta\tilde{C}p_A x_A)} \\ T(V_k = 0) = T_0^{(k)} \end{cases} \quad (\text{A63})$$

Energy Balance on CSTR

The energy balance on a generic adiabatic CSTR of the series is stated in the expressions reported in Equations (A64) and (A65):

$$\begin{aligned} F_A^{(0)} \left(\sum_{h=1}^k S_h \right) \left(\sum_{i=1}^n \left(\theta_i + \frac{v_i}{a} x_{A,0}^{(k)} \right) \tilde{H}_i(T_0^{(k)}) - \sum_{i=1}^n \left(\theta_i + \frac{v_i}{a} x_A^{(k)} \right) \tilde{H}_i(T^{(k)}) \right) = 0 \\ \sum_{i=1}^n \left(\theta_i + \frac{v_i}{a} x_{A,0}^{(k)} \right) \left[\Delta\tilde{H}_{f,i}^0 + \tilde{C}p_i(T_0^{(k)} - T_{ref}) \right] + \\ - \sum_{i=1}^n \left(\theta_i + \frac{v_i}{a} x_A^{(k)} \right) \left[\Delta\tilde{H}_{f,i}^0 + \tilde{C}p_i(T^{(k)} - T_{ref}) \right] = 0 \\ \sum_{i=1}^n \left[\left(\theta_i \Delta\tilde{H}_{f,i}^0 + \frac{v_i \Delta\tilde{H}_{f,i}^0}{a} x_{A,0}^{(k)} \right) + \left(\theta_i \tilde{C}p_i + \frac{v_i \tilde{C}p_i}{a} x_{A,0}^{(k)} \right) (T_0^{(k)} - T_{ref}) \right] + \\ - \sum_{i=1}^n \left[\left(\theta_i \Delta\tilde{H}_{f,i}^0 + \frac{v_i \Delta\tilde{H}_{f,i}^0}{a} x_A^{(k)} \right) + \left(\theta_i \tilde{C}p_i + \frac{v_i \tilde{C}p_i}{a} x_A^{(k)} \right) (T^{(k)} - T_{ref}) \right] = 0 \end{aligned} \quad (\text{A64})$$

$$\begin{aligned} \left[\left(\Delta\tilde{H}_{r,A}^0 x_{A,0}^{(k)} \right) + \left(\tilde{C}p_s + \Delta\tilde{C}p_A x_{A,0}^{(k)} \right) (T_0^{(k)} - T_{ref}) \right] + \\ - \left[\left(\Delta\tilde{H}_{r,A}^0 x_A^{(k)} \right) + \left(\tilde{C}p_s + \Delta\tilde{C}p_A x_A^{(k)} \right) (T^{(k)} - T_{ref}) \right] = 0 \end{aligned}$$

$$\begin{aligned} \left(\Delta\tilde{H}_{r,A}^0 x_{A,0}^{(k)} - \Delta\tilde{H}_{r,A}^0 x_A^{(k)} \right) + \tilde{C}p_s (T_0^{(k)} - T^{(k)}) \\ + \Delta\tilde{C}p_A x_{A,0}^{(k)} (T_0^{(k)} - T_{ref}) - \Delta\tilde{C}p_A x_A^{(k)} (T^{(k)} - T_{ref}) = 0 \end{aligned}$$

$$\tilde{C}p_s (T_0^{(k)} - T^{(k)}) + x_{A,0}^{(k)} \Delta\tilde{H}_{r,A}^0 (T_0^{(k)} - T^{(k)}) - x_A^{(k)} \Delta\tilde{H}_{r,A}^0 (T^{(k)} - T_{ref}) = 0$$

$$x_A^{(k)} \Delta\tilde{H}_{r,A}^0 (T^{(k)} - T_{ref}) = \tilde{C}p_s (T_0^{(k)} - T^{(k)}) + x_{A,0}^{(k)} \Delta\tilde{H}_{r,A}^0 (T_0^{(k)} - T^{(k)}) \quad (\text{A65})$$

$$x_A^{(k)} = \frac{\tilde{C}p_s}{\Delta\tilde{H}_{r,A}^0 (T^{(k)} - T_{ref})} (T_0^{(k)} - T^{(k)}) + \frac{\Delta\tilde{H}_{r,A}^0 (T_0^{(k)} - T^{(k)})}{\Delta\tilde{H}_{r,A}^0 (T^{(k)} - T_{ref})} x_{A,0}^{(k)}$$

The previous equation is simplified into Equation (A66) if the enthalpy of the reaction can be considered constant with temperature:

$$\left[x_{A,0}^{(k)} - x_A^{(k)} \right] = \frac{\tilde{C}p_s}{-\Delta\tilde{H}_{r,A}} (T_0^{(k)} - T^{(k)}) \quad (\text{A66})$$

Appendix A.5. Adiabatic-Stage Reactors with Distributed Interstage Feed

Appendix A.5.1. Mass Balances

Mass Balance on the Mixing Nodes

The mass balance of A on the mixing node before the entrance of each reactor allows us to express the inlet molar flow rate $F_{A,0}^{(k)}$ as a function of the outlet one exiting the preceding reactor $F_A^{(k-1)}$ and of the initial split flow rate $F_{A,S}^{(k)} = S_k F_A^{(0)}$ (Equation (A67)).

$$\begin{aligned} S_1 F_A^{(0)} &= F_{A,0}^{(1)} \\ F_A^{(1)} + S_2 F_A^{(0)} &= F_{A,0}^{(2)} \\ \dots \\ F_A^{(k-1)} + S_k F_A^{(0)} &= F_{A,0}^{(k)} \\ \dots \\ F_A^{(r-1)} + S_r F_A^{(0)} &= F_{A,0}^{(r)} \end{aligned} \quad (\text{A67})$$

The flow rates at the inlet and outlet of reactors are expressed in terms of conversion as follows (Equation (A68)):

$$\begin{aligned} F_{A,0}^{(1)} &= F_{A,0}^{*(1)} (1 - x_{A,0}^{(1)}) = S_1 F_A^{(0)} (1 - x_{A,0}^{(1)}) \\ F_A^{(1)} &= F_A^{*(1)} (1 - x_A^{(1)}) = S_1 F_A^{(0)} (1 - x_A^{(1)}) \\ F_{A,0}^{(2)} &= F_{A,0}^{*(2)} (1 - x_{A,0}^{(2)}) = (S_1 + S_2) F_A^{(0)} (1 - x_{A,0}^{(2)}) \\ F_A^{(2)} &= F_A^{*(2)} (1 - x_A^{(2)}) = (S_1 + S_2) F_A^{(0)} (1 - x_A^{(2)}) \\ \dots \\ F_{A,0}^{(k)} &= F_{A,0}^{*(k)} (1 - x_{A,0}^{(k)}) = \left(\sum_{h=1}^k S_h \right) F_A^{(0)} (1 - x_{A,0}^{(k)}) \\ F_A^{(k)} &= F_A^{*(k)} (1 - x_A^{(k)}) = \left(\sum_{h=1}^k S_h \right) F_A^{(0)} (1 - x_A^{(k)}) \\ \sum_{h=1}^r S_h &= 1 \end{aligned} \quad (\text{A68})$$

where the split ratios S_k are generally different from each other and can be subjected to optimisation to maximise the reactive network performance. Substituting the mass balances reported in Equation (A68) into Equation (A67), we obtain the inlet conversions $x_{A,0}$ as functions of the outlet ones (Equation (A69)), in analogy to the previously detailed case of recycle reactors.

$$\begin{aligned} x_{A,0}^{(1)} &= 0 \\ x_{A,0}^{(2)} &= \frac{S_1}{S_1 + S_2} x_A^{(1)} \stackrel{S_k=S}{=} \frac{S}{2S} x_A^{(1)} = \frac{1}{2} x_A^{(1)} \\ \dots \\ x_{A,0}^{(k)} &= \frac{\sum_{h=1}^{k-1} S_h}{\sum_{h=1}^k S_h} x_A^{(k-1)}, \quad x_{A,0}^{(k)} \Big|_{S_k=S} = \frac{k-1}{k} x_A^{(k-1)} \end{aligned} \quad (\text{A69})$$

Mass Balance on PFR

In the same way as performed before, we first write the general differential mass balance inside the generic PFR in terms of the key-species A (Equation (A70)):

$$\frac{dF_A}{dV} = r_A \quad (\text{A70})$$

Then, for each k -th reactor, we express the molar flow rate as a function of the respective conversion—defined as usual with respect to the molar flow rate of A in the absence of reaction (Equation (A71)):

$$\begin{aligned} S_1 F_A^{(0)} \frac{dx_A}{dV} &= (-r_A)_1 \\ (S_1 + S_2) F_A^{(0)} \frac{dx_A}{dV} &= (-r_A)_2 \\ &\dots \\ \left(\sum_{k=1}^{r-1} S_k \right) F_A^{(0)} \frac{dx_A}{dV} &= (-r_A)_{r-1} \\ F_A^{(0)} \frac{dx_A}{dV} &= (-r_A)_r \end{aligned} \quad (\text{A71})$$

From these expressions, we finally obtain the design equation for the generic k -th reactor written in its canonical integral form along with the necessary integration upper and lower limits (Equation (A72)):

$$\begin{aligned} \frac{V_{R_1}}{F_A^{(0)}} &= S_1 \int_0^{x_A^{(1)}} \frac{dx_A}{(-r_A)_{R_1}} \\ \frac{V_{R_2}}{F_A^{(0)}} &= (S_1 + S_2) \int_{\frac{S_1}{S_1+S_2} x_A^{(1)}}^{x_A^{(2)}} \frac{dx_A}{(-r_A)_{R_2}} \\ &\dots \\ \frac{V_{R_k}}{F_A^{(0)}} &= \left(\sum_{h=1}^k S_h \right) \int_{\frac{\sum_{h=1}^{k-1} S_h}{\sum_{h=1}^k S_h} x_A^{(k-1)}}^{x_A^{(k)}} \frac{dx_A}{(-r_A)_{R_k}} \end{aligned} \quad (\text{A72})$$

In the particular case in which all the split ratios are equal, we obtain the following simplified expressions (Equation (A73)):

$$\begin{aligned} S \int_0^{x_A^{(1)}} \frac{dx_A}{(-r_A)_{R_1}} &= \frac{V_{R_1}}{F_A^{(0)}} \\ 2S \int_{\frac{1}{2} x_A^{(1)}}^{x_A^{(2)}} \frac{dx_A}{(-r_A)_{R_2}} &= \frac{V_{R_2}}{F_A^{(0)}} \\ &\dots \\ kS \int_{\frac{k-1}{k} x_A^{(k-1)}}^{x_A^{(k)}} \frac{dx_A}{(-r_A)_{R_k}} &= \frac{V_{R_k}}{F_A^{(0)}} \end{aligned} \quad (\text{A73})$$

Mass Balance on CSTR

The mass balances on the CSTRs of the series are (Equation (A74)):

$$\begin{aligned} S_1 F_A^{(0)} - S_1 F_A^{(0)} (1 - x_A^{(1)}) &= (-r_A)_1 V_{R_1} \\ (S_1 + S_2) F_A^{(0)} (1 - x_{A,0}^{(2)}) - (S_1 + S_2) F_A^{(0)} (1 - x_A^{(2)}) &= (-r_A)_2 V_{R_2} \\ &\dots \\ \left(\sum_{h=1}^k S_h \right) F_A^{(0)} (1 - x_{A,0}^{(k)}) - \left(\sum_{h=1}^k S_h \right) F_A^{(0)} (1 - x_A^{(k)}) &= (-r_A)_k V_{R_k} \end{aligned} \quad (\text{A74})$$

After a further simplification, Equation (A74) becomes (Equation (A75)):

$$\begin{aligned} S_1 F_A^{(0)} x_A^{(1)} &= (-r_A)_1 V_{R_1} \\ (S_1 + S_2) F_A^{(0)} (x_A^{(2)} - x_{A,0}^{(2)}) &= (-r_A)_2 V_{R_2} \\ \dots \\ \left(\sum_{h=1}^k S_h \right) F_A^{(0)} (x_A^{(k)} - x_{A,0}^{(k)}) &= (-r_A)_k V_{R_k} \end{aligned} \quad (\text{A75})$$

Eliminating the inlet conversions $x_{A,0}$, we finally obtain (Equation (A76)):

$$\begin{aligned} S_1 F_A^{(0)} x_A^{(1)} &= (-r_A)_1 V_{R_1} \\ \left((S_1 + S_2) x_A^{(2)} - S_1 x_A^{(1)} \right) &= (-r_A)_2 \frac{V_{R_2}}{F_A^{(0)}} \\ \dots \\ \left[\left(\sum_{h=1}^k S_h \right) x_A^{(k)} - \left(\sum_{h=1}^{k-1} S_h \right) x_A^{(k-1)} \right] &= (-r_A)_k \frac{V_{R_k}}{F_A^{(0)}} \\ \frac{V_{R_k}}{F_A^{(0)}} &= \frac{\left[\left(\sum_{h=1}^k S_h \right) x_A^{(k)} - \left(\sum_{h=1}^{k-1} S_h \right) x_A^{(k-1)} \right]}{(-r_A)_k} \end{aligned} \quad (\text{A76})$$

If all split ratios are equal, we obtain (Equation (A77)):

$$\begin{aligned} S F_A^{(0)} x_A^{(1)} &= (-r_A)_1 V_{R_1} \\ S \left(2x_A^{(2)} - x_A^{(1)} \right) &= (-r_A)_2 \frac{V_{R_2}}{F_A^{(0)}} \\ \dots \\ S \left[kx_A^{(k)} - (k-1)x_A^{(k-1)} \right] &= (-r_A)_k \frac{V_{R_k}}{F_A^{(0)}} \\ \frac{V_{R_k}}{F_A^{(0)}} &= S \frac{\left[kx_A^{(k)} - (k-1)x_A^{(k-1)} \right]}{(-r_A)_k} \end{aligned} \quad (\text{A77})$$

Appendix A.5.2. Energy Balances

Energy Balance on the Mixing Nodes

Applying Equation (A41) to the generic branches entering and exiting the mixing node just before the k -th reactor, the energy balance on the k -th mixing node is written as a function of conversion as follows (Equation (A78)):

$$\begin{aligned} \sum_{i=1}^n F_i^{(k-1)} \tilde{H}_i(T^{(k-1)}) + F_{A,S}^{(k)} \tilde{H}_A(T_A^{(0)}) &= \sum_{i=1}^n F_{i,0}^{(k)} \tilde{H}_i(T_0^{(k)}) \\ F_i^{(k-1)} &= \begin{cases} F_A^{(0)} \left(\sum_{h=1}^{k-1} S_h \right) (1 - x_A^{(k-1)}), & i = A \\ F_A^{(0)} \left(\sum_{h=1}^{k-1} S_h \right) \left(\theta_{i \neq A}^{(k-1)} + \frac{v_i}{a} x_A^{(k-1)} \right), & i \neq A \end{cases} = \begin{cases} F_A^{(0)} \left(\sum_{h=1}^{k-1} S_h \right) (1 - x_A^{(k-1)}), & i = A \\ F_A^{(0)} \left(\theta_{i \neq A} + \sum_{h=1}^{k-1} S_h \frac{v_i}{a} x_A^{(k-1)} \right), & i \neq A \end{cases} \\ F_{i,0}^{(k)} &= \begin{cases} F_A^{(0)} \left(\sum_{h=1}^k S_h \right) (1 - x_{A,0}^{(k)}), & i = A \\ F_A^{(0)} \left(\sum_{h=1}^k S_h \right) \left(\theta_{i \neq A,0}^{(k-1)} + \frac{v_i}{a} x_{A,0}^{(k)} \right), & i \neq A \end{cases} = \begin{cases} F_A^{(0)} \left(\sum_{h=1}^k S_h \right) (1 - x_{A,0}^{(k)}), & i = A \\ F_A^{(0)} \left(\theta_{i \neq A} + \sum_{h=1}^k S_h \frac{v_i}{a} x_{A,0}^{(k)} \right), & i \neq A \end{cases} \end{aligned} \quad (\text{A78})$$

Developing Equation (A78) through the algebraic calculations detailed in Equations (A79)–(A84), we obtain Equation (A85), which states, as expected, that the resulting temperature $T_0^{(k)}$ exiting the mixing k -th node is comprised between the temperature entering the

node from the preceding reactor $T^{(k-1)}$ and the temperature of the split initial feed $T_A^{(0)}$ of the limiting reactant A.

$$\begin{aligned}
 F_A^{(k-1)} \tilde{H}_A(T^{(k-1)}) + \sum_{i=2}^n F_i^{(k-1)} \tilde{H}_i(T^{(k-1)}) + F_{A,S}^{(k)} \tilde{H}_A(T_A^{(0)}) &= \sum_{i=1}^n F_{i,0}^{(k)} \tilde{H}_i(T_0^{(k)}) \\
 F_A^{(0)} \left(\sum_{h=1}^{k-1} S_h \right) (1 - x_A^{(k-1)}) \tilde{H}_A(T^{(k-1)}) + F_A^{(0)} \sum_{i=2}^n \left[\theta_i + \left(\sum_{h=1}^{k-1} S_h \right) \frac{v_i}{a} x_A^{(k-1)} \right] \tilde{H}_i(T^{(k-1)}) \\
 + F_A^{(0)} S_k \tilde{H}_A(T^{(0)}) \\
 = F_A^{(0)} \left(\sum_{h=1}^k S_h \right) (1 - x_{A,0}^{(k)}) \tilde{H}_A(T_0^{(k)}) + F_A^{(0)} \sum_{i=2}^n \left[\theta_i + \left(\sum_{h=1}^k S_h \right) \frac{v_i}{a} x_{A,0}^{(k)} \right] \tilde{H}_i(T_0^{(k)}) \\
 \left(\sum_{h=1}^{k-1} S_h \right) \tilde{H}_A(T^{(k-1)}) - \left(\sum_{h=1}^{k-1} S_h \right) \tilde{H}_A(T^{(k-1)}) x_A^{(k-1)} \\
 + \sum_{i=2}^n \left[\theta_i \tilde{H}_i(T^{(k-1)}) + \left(\sum_{h=1}^{k-1} S_h \right) \frac{v_i}{a} \tilde{H}_i(T^{(k-1)}) x_A^{(k-1)} \right] \\
 + S_k \tilde{H}_A(T^{(0)}) \\
 = \left(\sum_{h=1}^k S_h \right) \tilde{H}_A(T_0^{(k)}) - \left(\sum_{h=1}^k S_h \right) x_{A,0}^{(k)} \tilde{H}_A(T_0^{(k)}) \\
 + \sum_{i=2}^n \left[\theta_i \tilde{H}_i(T_0^{(k)}) + \left(\sum_{h=1}^k S_h \right) \frac{v_i}{a} \tilde{H}_i(T_0^{(k)}) x_{A,0}^{(k)} \right]
 \end{aligned} \tag{A79}$$

$$\begin{aligned}
 \left(\sum_{h=1}^{k-1} S_h \right) [\Delta \tilde{H}_{f,A} + \tilde{C}p_A(T^{(k-1)} - T_r)] - \left(\sum_{h=1}^{k-1} S_h \right) [\Delta \tilde{H}_{f,A} + \tilde{C}p_A(T^{(k-1)} - T_r)] x_A^{(k-1)} \\
 + \sum_{i=2}^n \left[\theta_i [\Delta \tilde{H}_{f,i} + \tilde{C}p_i(T^{(k-1)} - T_r)] + \left(\sum_{h=1}^{k-1} S_h \right) \frac{v_i}{a} [\Delta \tilde{H}_{f,i} + \tilde{C}p_i(T^{(k-1)} - T_r)] x_A^{(k-1)} \right] \\
 + S_k [\Delta \tilde{H}_{f,A} + \tilde{C}p_A(T^{(0)} - T_r)] \\
 = \left(\sum_{h=1}^k S_h \right) [\Delta \tilde{H}_{f,A} + \tilde{C}p_A(T_0^{(k)} - T_r)] - \left(\sum_{h=1}^k S_h \right) x_{A,0}^{(k)} [\Delta \tilde{H}_{f,A} + \tilde{C}p_A(T_0^{(k)} - T_r)] \\
 + \sum_{i=2}^n \left[\theta_i [\Delta \tilde{H}_{f,i} + \tilde{C}p_i(T_0^{(k)} - T_r)] + \left(\sum_{h=1}^k S_h \right) \frac{v_i}{a} [\Delta \tilde{H}_{f,i} + \tilde{C}p_i(T_0^{(k)} - T_r)] x_{A,0}^{(k)} \right]
 \end{aligned} \tag{A80}$$

$$\begin{aligned}
 \left(\sum_{h=1}^{k-1} S_h \right) \Delta \tilde{H}_{f,A} + \left(\sum_{h=1}^{k-1} S_h \right) \tilde{C}p_A(T^{(k-1)} - T_r) + \left(\sum_{h=1}^{k-1} S_h \right) \frac{v_A}{a} \Delta \tilde{H}_{f,A} x_A^{(k-1)} + \left(\sum_{h=1}^{k-1} S_h \right) \frac{v_A}{a} \tilde{C}p_A x_A^{(k-1)} (T^{(k-1)} - T_r) \\
 + \left[\sum_{i=2}^n \theta_i \Delta \tilde{H}_{f,i} + (T^{(k-1)} - T_r) \sum_{i=2}^n \theta_i \tilde{C}p_i \right] + \left(\sum_{h=1}^{k-1} S_h \right) x_A^{(k-1)} \sum_{i=2}^n \frac{v_i}{a} \Delta \tilde{H}_{f,i} + (T^{(k-1)} - T_r) x_A^{(k-1)} \left(\sum_{h=1}^{k-1} S_h \right) \sum_{i=2}^n \frac{v_i}{a} \tilde{C}p_i \\
 + [S_k \Delta \tilde{H}_{f,A} + S_k \tilde{C}p_A(T^{(0)} - T_r)] \\
 = \left(\sum_{h=1}^k S_h \right) \Delta \tilde{H}_{f,A} + \left(\sum_{h=1}^k S_h \right) \tilde{C}p_A(T_0^{(k)} - T_r) + \left(\sum_{h=1}^k S_h \right) x_{A,0}^{(k)} \frac{v_A}{a} \Delta \tilde{H}_{f,A} + \left(\sum_{h=1}^k S_h \right) \frac{v_A}{a} \tilde{C}p_A x_{A,0}^{(k)} (T_0^{(k)} - T_r) \\
 + \sum_{i=2}^n \theta_i \Delta \tilde{H}_{f,i} + \sum_{i=2}^n \theta_i \tilde{C}p_i (T_0^{(k)} - T_r) + \left(\sum_{h=1}^k S_h \right) x_{A,0}^{(k)} \sum_{i=2}^n \frac{v_i}{a} \Delta \tilde{H}_{f,i} + \left(\sum_{h=1}^k S_h \right) x_{A,0}^{(k)} \sum_{i=2}^n \frac{v_i}{a} \tilde{C}p_i (T_0^{(k)} - T_r)
 \end{aligned} \tag{A81}$$

$$\begin{aligned}
 \left(\sum_{h=1}^{k-1} S_h \right) \Delta \tilde{H}_{f,A} + \left(\sum_{h=1}^{k-1} S_h \right) \tilde{C}p_A(T^{(k-1)} - T_r) + \left(\sum_{h=1}^{k-1} S_h \right) \frac{v_A}{a} \Delta \tilde{H}_{f,A} x_A^{(k-1)} + \left(\sum_{h=1}^{k-1} S_h \right) \frac{v_A}{a} \tilde{C}p_A x_A^{(k-1)} (T^{(k-1)} - T_r) \\
 + \sum_{i=2}^n \theta_i \Delta \tilde{H}_{f,i} + (T^{(k-1)} - T_r) \sum_{i=2}^n \theta_i \tilde{C}p_i + \left(\sum_{h=1}^{k-1} S_h \right) x_A^{(k-1)} \sum_{i=2}^n \frac{v_i}{a} \Delta \tilde{H}_{f,i} + (T^{(k-1)} - T_r) x_A^{(k-1)} \left(\sum_{h=1}^{k-1} S_h \right) \sum_{i=2}^n \frac{v_i}{a} \tilde{C}p_i \\
 + [S_k \Delta \tilde{H}_{f,A} + S_k \tilde{C}p_A(T^{(0)} - T_r)] \\
 = \left(\sum_{h=1}^k S_h \right) \Delta \tilde{H}_{f,A} + \left(\sum_{h=1}^k S_h \right) \tilde{C}p_A(T_0^{(k)} - T_r) + \left(\sum_{h=1}^k S_h \right) x_{A,0}^{(k)} \frac{v_A}{a} \Delta \tilde{H}_{f,A} + \left(\sum_{h=1}^k S_h \right) \frac{v_A}{a} \tilde{C}p_A x_{A,0}^{(k)} (T_0^{(k)} - T_r) \\
 + \sum_{i=2}^n \theta_i \Delta \tilde{H}_{f,i} + \sum_{i=2}^n \theta_i \tilde{C}p_i (T_0^{(k)} - T_r) + \left(\sum_{h=1}^k S_h \right) x_{A,0}^{(k)} \sum_{i=2}^n \frac{v_i}{a} \Delta \tilde{H}_{f,i} + \left(\sum_{h=1}^k S_h \right) x_{A,0}^{(k)} \sum_{i=2}^n \frac{v_i}{a} \tilde{C}p_i (T_0^{(k)} - T_r)
 \end{aligned} \tag{A82}$$

$$\begin{aligned}
& \left(\sum_{h=1}^{k-1} S_h \right) \tilde{C}p_A T^{(k-1)} - \left(\sum_{h=1}^{k-1} S_h \right) \tilde{C}p_A T_r + \left(\sum_{h=1}^{k-1} S_h \right) \frac{\nu_A}{a} \Delta \tilde{H}_{f,A} x_A^{(k-1)} \\
& + \left(\sum_{h=1}^{k-1} S_h \right) \frac{\nu_A}{a} \tilde{C}p_A x_A^{(k-1)} T^{(k-1)} - \left(\sum_{h=1}^{k-1} S_h \right) \frac{\nu_A}{a} \tilde{C}p_A x_A^{(k-1)} T_r \\
& + \sum_{i=2}^n \theta_i \Delta \tilde{H}_{f,i} + \sum_{i=2}^n \theta_i \tilde{C}p_i T^{(k-1)} - \sum_{i=2}^n \theta_i \tilde{C}p_i T_r + \left(\sum_{h=1}^{k-1} S_h \right) x_A^{(k-1)} \sum_{i=2}^n \frac{\nu_i}{a} \Delta \tilde{H}_{f,i} \\
& + x_A^{(k-1)} \left(\sum_{h=1}^{k-1} S_h \right) \sum_{i=2}^n \frac{\nu_i}{a} \tilde{C}p_i T^{(k-1)} - x_A^{(k-1)} \left(\sum_{h=1}^{k-1} S_h \right) \sum_{i=2}^n \frac{\nu_i}{a} \tilde{C}p_i T_r \\
& + \left[S_k \Delta \tilde{H}_{f,A} + S_k \tilde{C}p_A T^{(0)} - S_k \tilde{C}p_A T_r \right] \\
& = S_k \Delta \tilde{H}_{f,A} + \left(\sum_{h=1}^k S_h \right) \tilde{C}p_A T_0^{(k)} - \left(\sum_{h=1}^k S_h \right) \tilde{C}p_A T_r + \left(\sum_{h=1}^{k-1} S_h \right) x_A^{(k-1)} \frac{\nu_A}{a} \Delta \tilde{H}_{f,A} \\
& + \left(\sum_{h=1}^{k-1} S_h \right) \frac{\nu_A}{a} \tilde{C}p_A x_A^{(k-1)} T_0^{(k)} - \left(\sum_{h=1}^{k-1} S_h \right) \frac{\nu_A}{a} \tilde{C}p_A x_A^{(k-1)} T_r \\
& + \sum_{i=2}^n \theta_i \Delta \tilde{H}_{f,i} + \sum_{i=2}^n \theta_i \tilde{C}p_i \left(T_0^{(k)} - T_r \right) + \left(\sum_{h=1}^{k-1} S_h \right) x_A^{(k-1)} \sum_{i=2}^n \frac{\nu_i}{a} \Delta \tilde{H}_{f,i} \\
& + \left(\sum_{h=1}^{k-1} S_h \right) x_A^{(k-1)} \sum_{i=2}^n \frac{\nu_i}{a} \tilde{C}p_i T_0^{(k)} - \left(\sum_{h=1}^{k-1} S_h \right) x_A^{(k-1)} \sum_{i=2}^n \frac{\nu_i}{a} \tilde{C}p_i T_r
\end{aligned} \tag{A83}$$

$$\begin{aligned}
& \left(\sum_{h=1}^{k-1} S_h \right) \tilde{C}p_A T^{(k-1)} + \left[\tilde{C}p_s - \tilde{C}p_A \right] T^{(k-1)} + S_k \tilde{C}p_A T^{(0)} + T^{(k-1)} \left(\sum_{h=1}^{k-1} S_h \right) \Delta \tilde{C}p_A x_A^{(k-1)} \\
& = T_0^{(k)} \left[\left(\sum_{h=1}^{k-1} S_h \right) \tilde{C}p_A + S_k \tilde{C}p_A + \tilde{C}p_s - \tilde{C}p_A + \left(\sum_{h=1}^{k-1} S_h \right) \Delta \tilde{C}p_A x_A^{(k-1)} \right]
\end{aligned} \tag{A84}$$

$$T_0^{(k)} = \frac{\left[\left(\sum_{h=1}^{k-1} S_h \right) \tilde{C}p_A + \sum_{i=2}^n \theta_i \tilde{C}p_i + \left(\sum_{h=1}^{k-1} S_h \right) \Delta \tilde{C}p_A x_A^{(k-1)} \right] T^{(k-1)} + S_k \tilde{C}p_A T^{(0)}}{\left[\left(\sum_{h=1}^{k-1} S_h \right) \tilde{C}p_A + \sum_{i=2}^n \theta_i \tilde{C}p_i + \left(\sum_{h=1}^{k-1} S_h \right) \Delta \tilde{C}p_A x_A^{(k-1)} \right] + S_k \tilde{C}p_A}$$

$$T_0^{(k)} = \frac{w_1}{w_1 + w_2} T^{(k-1)} + \frac{w_2}{w_1 + w_2} T^{(0)}$$

$$\begin{aligned}
w_1 & \equiv \left[\left(\sum_{h=1}^{k-1} S_h \right) \tilde{C}p_A + \sum_{i=2}^n \theta_i \tilde{C}p_i + \left(\sum_{h=1}^{k-1} S_h \right) \Delta \tilde{C}p_A x_A^{(k-1)} \right] \\
w_2 & \equiv S_k \tilde{C}p_A
\end{aligned} \tag{A85}$$

If $\Delta \tilde{C}p_A$ can be neglected with respect to the other terms of the sum, we obtain Equation (A86):

$$\begin{aligned}
T_0^{(k)} & \cong \frac{\left[\left(\sum_{h=1}^{k-1} S_h \right) \tilde{C}p_A + \sum_{i=2}^n \theta_i \tilde{C}p_i \right] T^{(k-1)} + S_k \tilde{C}p_A T^{(0)}}{\left[\left(\sum_{h=1}^{k-1} S_h \right) \tilde{C}p_A + \sum_{i=2}^n \theta_i \tilde{C}p_i \right] + S_k \tilde{C}p_A} \\
T_0^{(k)} & \cong \frac{w_1}{w_1 + w_2} T^{(k-1)} + \frac{w_2}{w_1 + w_2} T^{(0)} \\
w_1 & \equiv \left[\left(\sum_{h=1}^{k-1} S_h \right) \tilde{C}p_A + \sum_{i=2}^n \theta_i \tilde{C}p_i \right] \\
w_2 & \equiv S_k \tilde{C}p_A
\end{aligned} \tag{A86}$$

If the split ratios are the same, we obtain the expression reported in Equation (A87):

$$T_0^{(k)} \Big|_{S_k=S} = \frac{\left[(k-1) S \tilde{C}p_A + \sum_{i=2}^n \theta_i \tilde{C}p_i \right] T^{(k-1)} + S \tilde{C}p_A T^{(0)}}{\left[(k-1) S \tilde{C}p_A + \sum_{i=2}^n \theta_i \tilde{C}p_i + S \tilde{C}p_A \right]} \tag{A87}$$

Energy Balance on PFR

The general energy balance for a PFR is recalled here from Equation (A19):

$$\frac{d}{dV} \left(\sum_{i=1}^n F_i \tilde{H}_i \right) = 0 \quad (\text{A88})$$

For the k -th reactor of the series, expressing this balance in terms of conversion, we obtain the final expression (Equation (A92)) through Equation (A89)–(A91):

$$\begin{aligned} \frac{d}{dV} \left(\left[F_A \left[\Delta \tilde{H}_{f,A}^0 + \tilde{C}p_A (T - T_{ref}) \right] \right] + \sum_{i=2}^n \left[F_i \left[\Delta \tilde{H}_{f,i}^0 + \tilde{C}p_i (T - T_{ref}) \right] \right] \right) = 0 \\ \frac{d}{dV} \left(\left[F_A^{(0)} \left(\sum_{h=1}^k S_h \right) (1 - x_A) \left[\Delta \tilde{H}_{f,A}^0 + \tilde{C}p_A (T - T_{ref}) \right] \right] + \right. \\ \left. + \sum_{i=2}^n \left[F_A^{(0)} \left(\theta_{i \neq A} + \sum_{h=1}^k S_h \frac{v_i}{a} x_A \right) \left[\Delta \tilde{H}_{f,i}^0 + \tilde{C}p_i (T - T_{ref}) \right] \right] \right) = 0 \end{aligned} \quad (\text{A89})$$

$$F_i = \begin{cases} F_A^{(0)} \left(\sum_{h=1}^k S_h \right) (1 - x_A), & i = A \\ F_A^{(0)} \left(\theta_{i \neq A} + \sum_{h=1}^k S_h \frac{v_i}{a} x_A \right), & i \neq A \end{cases}, \text{ in the } k\text{-th reactor}$$

$$\begin{aligned} \frac{d}{dV} \left(\left[F_A^{(0)} \left(\sum_{h=1}^k S_h \right) (1 - x_A) \left[\Delta \tilde{H}_{f,A}^0 + \tilde{C}p_A (T - T_{ref}) \right] \right] \right) + \\ \frac{d}{dV} \left(\sum_{i=2}^n \left[F_A^{(0)} \left(\theta_{i \neq A} + \sum_{h=1}^k S_h \frac{v_i}{a} x_A \right) \left[\Delta \tilde{H}_{f,i}^0 + \tilde{C}p_i (T - T_{ref}) \right] \right] \right) = 0 \end{aligned} \quad (\text{A90})$$

$$\begin{aligned} \left(F_A^{(0)} \left(\sum_{h=1}^k S_h \right) \sum_{i=1}^n \frac{v_i \tilde{H}_i(T)}{a} \left[\frac{dx_A}{dV} \right] \right) \\ + F_A^{(0)} \left(- \left(1 - \sum_{h=1}^k S_h \right) \tilde{C}p_A + \sum_{i=1}^n \theta_i \tilde{C}p_i + \left(\sum_{h=1}^k S_h \right) \sum_{i=1}^n \frac{v_i}{a} \tilde{C}p_i x_A \right) \frac{dT}{dV} = 0 \end{aligned}$$

$$\left[\tilde{C}p_S + \left(\sum_{h=1}^k S_h \right) x_A \Delta \tilde{C}p_A - \left(1 - \sum_{h=1}^k S_h \right) \tilde{C}p_A \right] \frac{dT}{dV} = \left(\sum_{h=1}^k S_h \right) \left[-\Delta \tilde{H}_{r,A} \right] \left[\frac{dx_A}{dV} \right] \quad (\text{A91})$$

$$\left[\begin{array}{c} \overbrace{\left(\tilde{C}p_S - \tilde{C}p_A \right) + \left(\sum_{h=1}^k S_h \right) \tilde{C}p_A}^{\text{Thermal contribution of the feed}} + \overbrace{\left(\sum_{h=1}^k S_h \right) x_A \Delta \tilde{C}p_A}^{\text{Non-linear contribution}} \\ \text{Contribution of the species other than A} \quad \text{Contribution of the species A} \end{array} \right] \frac{dT}{dV} = \overbrace{\left(\sum_{h=1}^k S_h \right) \left[-\Delta \tilde{H}_{r,A} \right] \left[\frac{dx_A}{dV} \right]}^{\text{Reaction Contribution}} \quad (\text{A92})$$

Energy Balance on CSTR

The energy balance on the k -th CSTR is obtained starting from Equation (A93):

$$\begin{aligned}
 & F_{A,0}^{(k)} [\tilde{H}_A(T_0^{(k)})] + \sum_{i=2}^n [F_{i,0}^{(k)}] [\tilde{H}_i(T_0^{(k)})] + \\
 & -F_A^{(k)} [\tilde{H}_A(T^{(k)})] - \sum_{i=2}^n [F_i^{(k)}] [\tilde{H}_i(T^{(k)})] = 0 \\
 & F_{i,0}^{(k)} = \begin{cases} F_A^{(0)} \left(\sum_{h=1}^k S_h \right) (1 - x_{A,0}^{(k)}), & i = A \\ F_A^{(0)} \left(\theta_{i \neq A} + \sum_{h=1}^k S_h \frac{v_i}{a} x_{A,0}^{(k)} \right), & i \neq A \end{cases} \quad (\text{A93}) \\
 & F_i^{(k)} = \begin{cases} F_A^{(0)} \left(\sum_{h=1}^k S_h \right) (1 - x_A^{(k)}), & i = A \\ F_A^{(0)} \left(\theta_{i \neq A} + \sum_{h=1}^k S_h \frac{v_i}{a} x_A^{(k)} \right), & i \neq A \end{cases}
 \end{aligned}$$

After some algebraic calculations (see Equations (A94), (A95) and (A99)), we can finally obtain the form reported in Equation (A96).

$$\begin{aligned}
 & F_A^{(0)} \left(\sum_{h=1}^k S_h \right) (1 - x_{A,0}^{(k)}) [\tilde{H}_A(T_0^{(k)})] \\
 & + \sum_{i=2}^n F_A^{(0)} \left(\theta_{i \neq A} + \sum_{h=1}^k S_h \frac{v_i}{a} x_{A,0}^{(k)} \right) [\tilde{H}_i(T_0^{(k)})] + \\
 & -F_A^{(0)} \left(\sum_{h=1}^k S_h \right) (1 - x_A^{(k)}) [\tilde{H}_A(T^{(k)})] + \\
 & - \sum_{i=2}^n F_A^{(0)} \left(\theta_{i \neq A} + \sum_{h=1}^k S_h \frac{v_i}{a} x_A^{(k)} \right) [\tilde{H}_i(T^{(k)})] = 0 \quad (\text{A94})
 \end{aligned}$$

$$\begin{aligned}
 & - \left(1 - \sum_{h=1}^k S_h \right) \tilde{H}_A(T_0^{(k)}) + \sum_{i=1}^n [\theta_{i \neq A} \tilde{H}_i(T_0^{(k)})] \\
 & + \sum_{i=1}^n \left[\left(\sum_{h=1}^k S_h \right) \frac{v_i}{a} \tilde{H}_i(T_0^{(k)}) x_{A,0}^{(k)} \right] + \\
 & \left(1 - \sum_{h=1}^k S_h \right) \tilde{H}_A(T^{(k)}) - \sum_{i=1}^n [\theta_{i \neq A} \tilde{H}_i(T^{(k)})] + \\
 & - \sum_{i=1}^n \left[\left(\sum_{h=1}^k S_h \right) \frac{v_i}{a} \tilde{H}_i(T^{(k)}) x_A^{(k)} \right] = 0 \quad (\text{A95})
 \end{aligned}$$

$$\begin{aligned}
 & \left[(\tilde{C}p_s - \tilde{C}p_A) + \left(\sum_{h=1}^k S_h \right) \tilde{C}p_A \right] (T_0^{(k)} - T^{(k)}) \\
 & + \left(\sum_{h=1}^k S_h \right) [x_{A,0}^{(k)} \Delta \tilde{H}_{r,A}(T_0^{(k)}) - x_A^{(k)} \Delta \tilde{H}_{r,A}(T^{(k)})] = 0 \quad (\text{A96})
 \end{aligned}$$

$$\begin{aligned}
 & \left[(\tilde{C}p_s - \tilde{C}p_A) + \left(\sum_{h=1}^k S_h \right) \tilde{C}p_A \right] (T_0^{(k)} - T^{(k)}) \\
 & + \left(\sum_{h=1}^k S_h \right) [x_{A,0}^{(k)} - x_A^{(k)}] \Delta \tilde{H}_{r,A} = 0 \quad (\text{A97})
 \end{aligned}$$

We remind that, from the previously obtained mass and energy balance on the mixing nodes, the following relationships hold for the inlet conversion and temperature (Equations (A98) and (A99)):

$$x_{A,0}^{(k)} = \frac{\sum_{h=1}^{k-1} S_h}{\sum_{h=1}^k S_h} x_A^{(k-1)} \quad (\text{A98})$$

$$T_0^{(k)} \cong \frac{\left[\left(\sum_{h=1}^{k-1} S_h \right) \tilde{c}p_A + \sum_{i=2}^n \theta_i \tilde{c}p_i \right] T^{(k-1)} + S_k \tilde{c}p_A T^{(0)}}{\left[\left(\sum_{h=1}^{k-1} S_h \right) \tilde{c}p_A + \sum_{i=2}^n \theta_i \tilde{c}p_i \right] + S_k \tilde{c}p_A} \quad (\text{A99})$$

Substituting Equations (A98) and (A99) into Equation (A97), we obtain the following expression (Equation (A100)):

$$\begin{aligned} & \left(\sum_{h=1}^k S_h \right) \left[x_A^{(k)} - x_A^{(k-1)} \right] + S_k \left[x_A^{(k-1)} - \underbrace{x_A^{(0)}}_{=0} \right] \\ &= \frac{\left(\sum_{h=1}^k S_h \right) \tilde{c}p_A + (\tilde{c}p_s - \tilde{c}p_A)}{(-\Delta \tilde{H}_{r,A})} \left(T^{(k)} - T^{(k-1)} \right) \\ &+ \frac{S_k \tilde{c}p_A}{(-\Delta \tilde{H}_{r,A})} \left(T^{(k-1)} - T^{(0)} \right) \end{aligned} \quad (\text{A100})$$

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