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# Data Reconciliation for Chemical Reaction Systems Using Vessel Extents and Shape Constraints

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**Abstract**

Concentrations measured during the course of reactions are typically corrupted by noise. Data reconciliation techniques improve the accuracy of measurements by using redundancies in the material and energy balances expressed as relationships between measurements. Since in the absence of kinetic models these relationships cannot integrate information regarding past measurements, they are expressed in the form of algebraic constraints. This paper shows that, even in the absence of a kinetic model, one can use shape constraints to relate measurements at different time instants, thereby improving the accuracy of reconciled estimates. The construction of shape constraints depends on the operating mode of the reactor. Moreover, it is shown that the representation of the reaction system in terms of vessel extents helps identify additional shape constraints. A procedure for deriving shape constraints from measurements is also described. Data reconciliation using both numbers of moles and extents is illustrated via a simulated case study.

**Keywords:** Chemical reaction systems, Data reconciliation, Variants and Invariants, Extents, Shape constraints.

## 1 Introduction

Many (bio-)chemical industries use chemical reaction systems to produce marketable products from raw materials [1, 2]. The conversion to products can take place in a single phase or in multiple phases with mass transfer between phases [3]. Moreover, the reaction systems can also involve inlet and outlet streams to feed reactants and remove the products. Process monitoring, control and optimization are important techniques for the safe and efficient operation of these reaction processes [4].

Traditionally, process monitoring, control and optimization are performed using kinetic models describing the behavior of the underlying chemical reaction system [5, 6, 7]. The term "process" or "plant" is used to describe the reaction system in production under real operating conditions. Developing a kinetic model for a reaction system may be complex and time consuming, and it typically uses measurements from laboratory experiments [2, 8, 9]. In addition, if the experimental conditions used to identify the model do not span the entire operating domain, the resulting model may fail to describe the reality of the plant. This has led researchers to develop approaches directly based on the analysis of plant data in real time [10, 11]. The quality of the kinetic models and the efficiency of these data-driven techniques