# Operability and Safety Considerations in Process Intensification

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**Abstract:** The importance of considering operability, control, and safety criteria in the analysis and design of process intensification configurations is discussed in this paper. We first rigorously analyze the loss of degrees of freedom and role of constraints in intensified systems comparing with their conventional process counterparts. A comparison study on inherent safety metrics in reactive distillation process is then presented to stress the need for new safety metrics at early design stage. To address these operability and safety challenges, we highlight a framework for systematic integration of operability, safety, and control to synthesize operable process intensification systems.

Keywords: Operability, Control, Safety, Process Intensification, Design & Control

# 1. INTRODUCTION

Facing a highly competitive global market with increasing awareness on environmental and safety issues, chemical production is making its way towards a paradigm shift more efficient and more sustainable (Avraamidou et al., 2019). Process intensification (PI) is regarded as a promising means to pursue this structural transformation, by boosting process and energy efficiency, enhancing process profitability and safety, reducing waste and emissions via innovative process solutions (Stankiewicz and Moulijn, 2000; Bielenberg and Palou-Rivera, 2019). While many PI technologies have been developed and compared with existing conventional process alternatives, computer-aided methods and tools to systematically derive operable and safe intensified designs are still lacking (Tian et al., 2018).

In this paper, we first discuss operability and safety challenges in process intensification (Tian and Pistikopoulos, 2019). Taking an intensified reactive distillation process and a conventional reactor-distillation-recycle process as an example, we rigorously analyze the impact on operability of key factors such as (i) degrees of freedom (DOFs), and (ii) role of model constraints. We also present a comparison study on different inherent safety metrics to demonstrate the need for a new metric to ensure valid and consistent evaluation of safety performance.

To address these challenges, we present a systematic framework for the analysis and synthesis of operable process intensified systems which includes: (i) phenomenabased synthesis representation, (ii) advanced control, operability, and safety metrics to address the unique operational characteristics in intensified designs under both steady-state and dynamic conditions, and (iii) integration with the Parametric Optimisation and Control (PAROC) platform to deliver verifiable and operable PI designs.

# 2. OPERABILITY & SAFETY CHALLENGES IN PI

Compared to conventional unit operations, intensified process structures pose unique and formidable operational challenges as detailed below, which necessitate the development of model-based metrics and tools to assess their operability, safety, and control at early design stage.

- Loss of DOFs due to tight integration By integrating multiple process steps (or functions) into a single intensified unit, the manipulated variables from the original flowsheet internal streams (i.e., non-inlet or outlet stream to the overall process) are no longer available for control (Baldea, 2015).
- Reduced operating window due to shared operating conditions of multi-phenomena For example, in reactive distillation, reaction and separation occur at the same pressure and temperature conditions in a single unit (Kiss et al., 2018).
- Highly nonlinear dynamic behaviour due to complex interplay between multi-phenomena This may possibly lead to the existence of multiple steady-states with different conversions under the same operating conditions (Nikačević et al., 2012).
- **Periodic operation for intensification** Periodic operating schemes (e.g., pressure swing adsorption) are more difficult to operate and control, particularly due to the lack of a steady-state operating point and nonlinear behaviour (Khajuria and Pistikopoulos, 2013).
- Insufficient design and operating information for safety assessment in novel PI designs Classical safety evaluation methods are often based on semi-heuristics and are employed as posterior evaluation tool which require detailed equipment/plant design and operating information (Etchells, 2005).

### 3. LOSS OF DEGREES OF FREEDOM

In this section, we will compare the degrees of freedom (DOFs) in an intensified reactive distillation process and a conventional reactor-distillation-recycle process, as illustrated in Figs. 1 and 2. DOFs will be classified as the following three types (Nikačević et al., 2012): (i) thermodynamic DOFs – which give the number of independent intensive system properties such as pressure and temperature, (ii) design DOFs – which are the number of independent geometrical properties available for process design, and (iii) operational DOFs - which identify the number of independent process variables that can be manipulated for process control and operation. Thermodynamic DOFs and design DOFs implicitly affect operability via "the impact of design on operability", while operational DOFs directly affect the available controller manipulated variables. In what follows, three types of process models are considered to detail the changes of DOFs at different modeling stages, namely: (i) steady-state modeling, (ii) dynamic modeling, and (iii) superstructure-based synthesis modeling.



Fig. 1. Intensified reactive distillation process.



Fig. 2. Conventional reactor-distillation-recycle process

### 3.1 Steady-State Modeling

Hereafter we consider a generalized process system with NC components, 1 feed stream, and 2 product streams. Both the reactive distillation column and conventional distillation column (Figs. 1 and 2) are assumed to have Ntray column trays. The (reactive) distillation model is built on that presented in Viswanathan and Grossmann (1993) with a superstructure-based mixed-integer formulation for column design optimization. The degrees of freedom in these two processes are presented in detail in Tables 1 and 2 with respect to their thermodynamic, design, and operational roles. As can be noticed, the intensified reactive distillation process suffers from the loss of 7 DOFs due to:

- (i) Highly coupled thermodynamic phenomena which reduces the operation window of process temperature and pressure
- (ii) Decreased number of processing units with corresponding design and operational DOFs
- (iii) Vanishing of interconnecting streams as potential manipulation points.

	Variable	Number of DOFs
	Stage pressures	Ntray
Thermodynamic DOFs	Reboiler pressure	1
	Condenser pressure	1
	Feed tray structure	Ntray - 1
Design DOFs	Reflux tray structure	Ntray - 1
	Catalyst load	Ntray
	Feed conditions	NC + 3
	(i.e. flowrate, temperature,	
Operational DOF	pressure, compositions)	
Operational DOFS	Reflux ratio, Boilup ratio	choose 2
	Bottoms rate, Distillate rate,	
	Reboiler duty, Condenser duty	
Sum		4Ntray + NC + 5

Table 1. Steady-state modeling DOFs – Reactive distillation

Table 2. Steady-state modeling DOFs – Reactor-distillation-recycle.

		Variable	Number of DOFs
	Distillations	s: Stage pressures	$Ntray \times 2$
Thermodynamic		Reboiler pressure	$1 \times 2$
DOFs		Condenser pressure	$1 \times 2$
	Reactor:	Temperature, Pressure	2
	Distillations	s: Feed tray structure	$(Ntray - 1) \times 2$
Design DOFs		Reflux tray structure	$(Ntray - 1) \times 2$
	Reactor:	Volume	1
	Feed conditions		NC + 3
Operational	Distillations: Reflux ratio,		choose $2 \times 2$
DOFs	Boilu	p ratio, Bottoms rate,	
	Disti	llate rate, Reboiler duty,	
	Cond	enser duty	
	Reactor:	Outlet flowrate	1
	Flowsheet:	Recycle ratio	1
Sum			6Ntray + NC + 12

### 3.2 Dynamic Modeling

Similarly with Section 3.1, we perform DOF analysis but based on dynamic high-fidelity modeling. The (reactive) distillation column is described using the mixedinteger dynamic models presented in Bansal et al. (2000). Dynamic models consist of more modeling constraints and process variables than steady-state models in order to accurately capture process dynamic behaviours. For distillation-based systems, column mass/energy holdups, pressure driving forces, and sizing correlations are of particular importance for dynamic considerations. As can be seen in Tables 3 and 4, the reactive distillation process still features the loss of DOFs in the context of its conventional process alternative. The internal process recycle ratio becomes no long available for control. Also the DOFs are lost for reactor design and operation (i.e., liquid level, diameter, pressure, temperature), causing a reduced design and operation window in such an intensified process.

	Variable	Number of DOFs
Thermodynamic DOFe	Reboiler pressure	1
Thermodynamic DOFs	Condenser pressure	1
	Feed tray structure	Ntray - 1
	Reflux tray structure	Ntray - 1
Desim DOF	Diameter, weir height, tray spacing	3
Design DOF's	Reflux drum diameter & length	2
	Reboiler diameter & length	2
	Catalyst load	Ntray
	Feed conditions	NC + 3
Operational DOFs	Reflux ratio, Boilup ratio	choose 2
	Bottoms rate, Distillate rate,	
	Reboiler duty, Condenser duty	
Sum		2Ntray + NC + 12

# Table 3. Dynamic modeling DOFs – Reactive distillation.

### Table 4. Dynamic modeling DOFs – Reactor-distillation-recycle.

	Variable	Number of DOFs
	Distillations: Reboiler pressure	$1 \times 2$
Thermodynamic	Condenser pressure	$1 \times 2$
DOFs	Reactor: Temperature	1
	Pressure	1
	Distillations: Feed tray structure	$(Ntray - 1) \times 2$
	Reflux tray structure	$(Ntray - 1) \times 2$
Design DOFs	Diameter, weir height, tray spacing	$3 \times 2$
Design DOFs	Reflux drum diameter & length	$2 \times 2$
	Reboiler diameter & length	$2 \times 2$
	Reactor: Height & Diameter	2
	Feed conditions	NC + 3
	Distillations: Reflux ratio, Boilup ratio	choose $2 \times 2$
Operational	Bottoms rate, Distillate rate,	
DOFs	Reboiler duty, Condenser duty	
	Reactor: Outlet flowrate	1
	Flowsheet: Recycle ratio	1
Sum		4Ntray + NC + 27

3.3 Superstructure-based Synthesis Modeling

To fully exploit the potential to discover innovative process options, some recent works for the optimization and synthesis of PI processes are going beyond unit operation concepts and exploring more generalized phenomena-based representation approaches to derive intensified designs without any pre-postulating any plausible equipment or flowsheets (Demirel et al., 2017; Tula et al., 2019; da Cruz and Manousiouthakis, 2019).

In this section, we investigate the DOFs at this synthesis level based on the Generalized Modular Representation Framework (GMF) developed in our previous works (Papalexandri and Pistikopoulos, 1996; Tian and Pistikopoulos, 2018). As depicted in Fig. 3, GMF utilizes two types of phenomenological modules to represent chemical processes, i.e. a pure heat exchange module and a mass/heat exchange module. A superstructure network is constructed to allow for all possible interconnections between these GMF modules to enable an enriched design space.



Fig. 3. GMF modular superstructure for process synthesis representation.

To provide a more intuitive example for this case, given an olefin metathesis process which involves 1 feed stream, 2 product streams, 3 components (i.e., pentene, butene, hexene), 5 GMF mass/heat exchange modules are employed to encapsulate the plausible process alternatives. This gives a total number of 493 equality constraints, 459 inequality constraints, 675 continuous variables, and 217 integer variables – resulting in 182 degrees of freedom based on a combinatorial superstructure representation.

However, many of these DOFs will appear or disappear with the selection of binary variables. GMF synthesis optimization can systematically generate intensified process solutions such as reactive distillation (Fig. 4) or conventional process alternatives such as reactor-distillationrecycle (Fig. 5). The DOF analysis on these configurations becomes identical with that of steady-state and dynamic modeling, with more DOFs in the latter process due to reactor design and recycle flow.



Fig. 4. GMF representation – Reactive distillation.



Fig. 5. GMF representation – Reactor-distillation-recycle.

# 4. ROLE OF CONSTRAINTS

From a model-based perspective, any operability, safety, or control concerns can be viewed as violation of model constraints. Thus in this section, we compare the above introduced reactive distillation process and CSTR-distillationrecycle process with respect to model constraints.

### 4.1 Steady-State and Dynamic Modeling

The differences of model constraints in the reactive distillation and the CSTR-distillation-recycle process majorly lie in the following inequality constraints:

- (i) Flowrate bounds The conventional process has additional flowrate bounds on external flows (e.g., recycle stream, connecting stream between reactor and distillation columns). However, in the case of reactive distillation, these flows are converted to internal flows inside the unit constrained by flooding and entrainment calculations incorporated in high fidelity dynamic modeling.
- (ii) Temperature/Pressure bounds The temperature and pressure bounds are different for these two processes. For example, the operating window of reactive distillation is a subset of the reactor operating window as well as of the distillation operating window, since it needs to achieve the desired reactive conversion and separation specification under a unified temperature/pressure profile.

### 4.2 Superstructure-based Synthesis Modeling

The differences in representing intensified process tasks (e.g., reactive separation) and conventional process tasks (e.g., reaction, separation) also lie in inequality model constraints:

# (i) Driving force constraints to characterize mass transfer feasibility

Separation task

$$\left(f^{LO}x_i^{LO} - f^{LI}x_i^{LI}\right) \times \ln\left[\frac{\gamma_i^L x_i^L P_i^{\operatorname{sat},L}}{\phi_i^V x_i^V P_{tot}}\right] \le 0 \quad (1)$$

Reaction task

$$(f^{LO}x_i^{LO} - f^{LI}x_i^{LI}) \times \sum_i \sum_k \left[\frac{\nu_{ik}\Delta G_i^f}{RT} + \nu_{ik} \ln(\phi_i^V x_i^V P_{tot})\right] \frac{\partial \epsilon_k}{\partial n_i^L} \le 0 \quad (2)$$

Reactive separation task

$$(f^{LO}x_i^{LO} - f^{LI}x_i^{LI}) \times (\ln\left[\frac{\gamma_i^L x_i^L P_i^{\operatorname{sat},L}}{\phi_i^V x_i^V P_{tot}}\right] + \sum_i \sum_k \left[\frac{\nu_{ik}\Delta G_i^f}{RT} + \nu_{ik} \ln(\phi_i^V x_i^V P_{tot})\right] \frac{\partial \epsilon_k}{\partial n_i^L}) \le 0$$
(3)

### (ii) Phase defining constraints to characterize operation phase conditions

Separation & Reactive separation tasks with coexisting liquid and vapor phases

liquid phase: 
$$\sum_{i} \gamma_{i} P_{i}^{\text{sat}} x_{i} / P_{tot} \leq 1$$
  
vapor phase: 
$$\sum_{i} P_{tot} y_{i} / \gamma_{i} P_{i}^{\text{sat}} \leq 1$$
 (4)

Reaction task with a single liquid phase (vanishing of vapor phase for operation)

liquid phase: 
$$\sum_{i} \gamma_i P_i^{\text{sat}} x_i / P_{tot} \le 1$$
 (5)

In the above modeling equations, f denotes flow rate, x represents molar fraction, i defines the component set, n gives the molar amount, L refers to liquid phase, gamma and  $\phi$  are respectively activity and fugacity coefficients,  $P^{\text{sat}}$  is saturated vapor pressure, T gives temperature, P denotes pressure, R is ideal gas constant,  $\nu$  is stoichiometric coefficient, and  $\Delta G^f$  stands for standard Gibbs function of formation.

### 5. INHERENT SAFETY METRICS

To evaluate inherent safety performance as part of early design, several key open questions need to be addressed:

- Development of standardized metrics to quantify inherent safety performance based on limited information available at early design stage
- Integration of inherent safety metrics into modelbased synthesis/design procedure
- Quantitative decision making to design or retrofit processes with enhanced safety performance.

In this section, we present a comparative study of three available inherent safety metrics for inherent safety evaluation of a methyl tert-butyl ether (MTBE) reactive distillation process. These approaches are respectively: (i) Risk analysis (Nemet et al., 2018), (ii) DOW indices (AIChE, 2010; Marshall and Mundt, 1995), and (iii) SWeHI index (Khan et al., 2001). Their performance are tested to reflect two major inherent safety principles (i.e., minimization, attenuation) with respect to fire & explosion hazard and health hazard.

### 5.1 Minimization

To test the above safety metrics against the minimization of process inventory, we consider three reactive distillation columns (i.e., A, B, C) producing MTBE from methanol and isobutylene with different capacities resulted by different column diameters. The other design and operating parameters remain the same.

Given an instantaneous release of total column inventory, the inherent safety performances of Column A, B, and C are assessed using risk analysis approach, DOW indices, and SWeHI index in terms of toxicity and fire & explosion (F&E). Evaluation results are presented below in Table 5. As can be noticed, all the metrics suggest the same ranking order as: Column A inherently safer than B and also than C, which aligns with the well-accepted statement that "less is safer".

Note that it may not be necessary to compare the absolute result values given by these different approaches since they are estimating for different damage scenarios. However, the sensitivity of each metric with respect to the change of inventory holdup is of interest. For example, Column C has an inventory more than 10 times of that in Column A. Risk analysis approach identified around 10 times increase of both fire & explosion risk and toxicity risk – which scale in a nearly linear fashion with the inventory. However, DOW F&EI gives very similar Radius of Exposure, hardly reflecting the significant scaling up of equipment size. The other DOW CEI & SWeHI indices give around 3 times larger hazard radius.

Table	5.	Inherent	safety	comparison	study:
		Minim	ization	effects.	

		А	В	С	$\begin{array}{c} {\rm Rank} \\ {\rm (unsafer} \\ \rightarrow {\rm safer}) \end{array}$
Invento	ry (kg)	145	1009	1744	
	Risk	4.73e-7	30.6e-7	42.5e-7	C < B < A
F & E	F&EI	$17.7 \mathrm{m}$	$20.6 \mathrm{m}$	$22.1 \mathrm{m}$	C < B < A
	SWeHI	$35.2 \mathrm{m}$	$67.3 \mathrm{m}$	$80.7 \mathrm{m}$	C < B < A
Toxicity	Risk	3.6e-5	24.6e-5	52.8e-5	C < B < A
	CEI	$73.1 \mathrm{m}$	$184.8~\mathrm{m}$	$239.6~\mathrm{m}$	C < B < A
	SWeHI	$46.7~\mathrm{m}$	$106.9~\mathrm{m}$	$135.0~\mathrm{m}$	C < B < A

### 5.2 Attenuation

To test these safety metrics against the attenuation of process operating conditions, we consider another three MTBE reactive distillation columns (i.e., a, b, c) with different operating pressures. The other design and operating parameters remain the same. Evaluation results are shown below in Table 6. For fire & explosion hazard, it can be seen that the increase of pressure is not well captured by all these approaches since they give very similar evaluation results. With respect to toxicity health hazard, these approaches are suggesting inconsistent ranking orders, and there is a conflict in ranking Column a to be the most safer process (i.e., risk analysis and CEI) or the most unsafer one (i.e., SWeHI).

Table 6. Inherent safety comparison study:Attenuation effects.

		a	b	с	Rank (unsafer
					$\rightarrow$ sater)
Pressure	e (atm)	1	6	11	
F & E	Risk	30.6e-7	80.5e-7	86.3e-7	c < b < a
	F&EI	$20.6 \mathrm{m}$	23.3  m	$23.9 \mathrm{m}$	$c\approx b < a$
	SWeHI	$67.3 \mathrm{m}$	$69.1 \mathrm{m}$	$69.3 \mathrm{m}$	$c\approx b < a$
Toxicity	Risk	24.6e-5	196e-5	168e-5	b < c < a
	CEI	$184.8~\mathrm{m}$	$212.9~\mathrm{m}$	$218.7~\mathrm{m}$	c < b < a
	SWeHI	$106.9 \mathrm{m}$	$98.5 \mathrm{m}$	100.5  m	a < c < b

### 5.3 Some remarks for safety metrics

It has been shown that none of these metrics can effectively reflect the minimization and attenuation impacts on inherent safety performances. Moreover, inconsistent evaluation results have been observed, thus making it ambiguous to determine the inherent safety performance of a certain design configuration. In this context, a new safety metric (or index) is highly necessitated and recommended to correctly and consistently evaluate inherent safety performance of different process options at this conceptual design stage.

### 6. A SYSTEMATIC FRAMEWORK FOR SYNTHESIS OF OPERABLE PI SYSTEMS

In the previous sections, we have discussed operability, safety, control challenges in process intensification systems. Towards a holistic approach to synthesize PI processes with operability, safety, and control considerations consistently through both steady-state design and dynamic operation, we have recently proposed a systematic framework as show in Fig. 6 (Tian et al., 2020). A stepby-step procedure is summarized below:

Step 1 – Process synthesis and intensification with the phenomena-based Generalized Modular Representation Framework to generate optimal and intensified process alternatives.

Step 2 – Flexibility and risk analysis to ensure that the derived intensified structures are operable and inherent safer at the conceptual design stage.

Step 3 – Design of explicit model-based predictive controller via the PAROC framework to ensure feasible operation under process disturbance and uncertainty.

Step 4 – Simultaneous design and control optimization to generate operable and optimal intensified designs.



Fig. 6. The proposed framework (adapted from Tian et al. (2020)).

Particularly for dynamic operation and model predictive control, we employ the PAROC framework (Pistikopoulos et al., 2015), which provides a unified framework and software platform for the design, operational optimization. and explicit model predictive control of chemical processes leveraging advanced multi-parametric programming algorithms. As depicted in Fig. 7, some of key features of the PAROC framework include: (i) high fidelity modeling based on first-principles to ensure accurate description of process dynamic behaviour; (ii) exact MPC solution obtained via offline multi-parametric quadratic programming; (iii) design-dependent mp-MPC controller derivation to handle process operation under different designs: and (v) implementation of (mixed-integer) dynamic optimization integrating high fidelity model and MPC controller to determine optimal design with optimal control actions. The framework has also been extended to incorporate operability and safety metrics (Tian et al., 2020).

### 7. CONCLUSION

In this work, we have discussed several key open questions on operability and safety in process intensification. We have also presented rigorous analysis on degrees of freedom, role of model constraints, and inherent safety metrics to highlight the importance of developing operability, control, and safety metrics and tools for PI assessment. A framework is introduced to systematically synthesize novel



Fig. 7. The PAROC framework (adapted from Pistikopoulos et al. (2015)).

intensified configurations with guaranteed operational performances. Ongoing work focuses on model-based analysis of synthesis and control operating windows of intensified and conventional systems towards a formal theory of operability in process intensification.

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