An optimal control approach to considering uncertainties in kinetic parameters in the maintenance scheduling and production of a process using decaying catalysts

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Abstract

This article presents a novel approach for optimising maintenance scheduling and production in a process using decaying catalysts while considering uncertainties in the kinetic parameters involved. The approach formulates this problem as a multistage mixed-integer optimal control problem (MSMIOCP) and uses a solution methodology that can offer a number of potential advantages over conventional methodologies. The solution methodology involves using a multiple scenario approach to consider parametric uncertainties and formulating a stochastic version of the MSMIOCP, which is solved as a standard nonlinear optimisation problem using a technique developed in a previous work. The proposed formulation and solution methodology are applied to identify the effects on the optimal process operation, of individual uncertainty of each parameter, of simultaneous uncertainty of all parameters and of the number of scenarios generated, as four case studies. The results obtained provide insights into these aspects and indicate the approach's capability to

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solve this problem.

Keywords: Uncertainties; Optimal control problem; Mixed-integer optimisation; Catalyst replacement; Scheduling; Production planning

1. Introduction and literature review

In industrial processes that use predictions from kinetic rate equations, the making of decisions for optimal functionality faces significant challenges due to uncertainties regarding the values of the parameters used in those equations. As they are experimentally obtained, these parameters values are susceptible to a degree of uncertainty because of inevitable inaccuracies arising from measurement errors, estimation errors, interpolation and extrapolation errors etc. In order to incorporate such uncertainties, these kinetic parameters are considered as taking values within a certain range, rather than be regarded as fixed constants.

In industrial processes producing commercial products using catalysts that decay in performance with time, the uncertainties in kinetic parameters manifest in the rate equations for the product formation reaction and catalyst deactivation. These industries face complex economic challenges because catalyst deactivation is inevitable and causes a loss in process productivity and revenue. In order to restore process performance, a maintenance action is required in which the reactor is shut down to replace the decayed catalyst with a fresh catalyst that has full activity. Such a maintenance action is called a catalyst replacement or a catalyst changeover operations. While this maintenance action improves product yield, there are negative effects involved such as a loss of production time, and energy and labour costs.

Thus, while frequently replacing catalyst loads can ensure high productivity, it also involves increased maintenance costs and loss of production time. An efficient schedule for catalyst replacements is needed to address this trade-off. Other considerations also have to be managed in tandem with deciding the catalyst replacement schedule such as the optimal operating conditions of the reactor, as well as the product inventory and sales to adequately meet time-varying demand.

Since the outputs of the kinetic models form the basis for making optimal decisions, there can be many implications to not considering uncertainties in kinetic parameters. For instance, uncertainty in the rate of product formation or catalyst decay can result in variable and unpredictable production times and yields. This can create difficulties in identifying the optimal maintenance schedules, operating conditions, and the appropriate production amounts and inventory levels to effectively meet product demand. An uncertainty in the rate of catalyst decay could also lead to the catalyst being used beyond its recommended lifespan, which could affect the durability of the reactor and threaten safe process operation. Hence, it is critical to take uncertainty in kinetic parameters into account while optimising process operations.

A search through literature revealed a very limited set of studies that considered uncertainty in kinetic parameters while optimising maintenance scheduling and production planning in processes using decaying catalysts. Only two such studies have been found and these have been based on online or data-driven methods of optimisation.

One is a work by Lim et al. (2009), which proposed a proactive scheduling strategy, that used comparisons between model predictions and actual measurements, to handle uncertainties in coke thickness and growth rates in the scheduling of decoking operations in a naptha cracking furnace system. The other work is by Jahandideh et al. (2019), which optimised scheduling of decaying catalysts and production in a process, while considering uncertain decay rates, by formulating this problem as a semi-Markov decision process.

However, the use of online methods, as in the aforementioned literature, does not enable a sensitivity analysis, or a quantification of the impact of uncertainty in a particular parameter, to be performed. In addition, these methods cannot identify the effect of uncertainties before the process begins execution. Obtaining prior predictions of the optimal maintenance schedules and operating conditions and the expected profits, while considering uncertainties, can aid in improving investment and operating decisions. To fulfil such purposes, preventive methods for handling uncertainties need to be used.

The popular preventive methods for scheduling optimisation under uncertainty include stochastic programming, fuzzy programming, robust optimisation and parametric programming (Li and Ierapetritou, 2008a). The use of one of these techniques in combination with a mixed-integer formulation represent the conventional methodology of solving scheduling problems involving parametric uncertainties. There are several publications that have used such methodologies to optimise scheduling in varied processes while considering uncertainty in parameters such as processing times, demand and prices, to name a few, and a literary review of such publications can be found in Aytug et al. (2005), Li and Ierapetritou (2008a) and Verderame et al. (2010).

However, no work exists that has used one of the conventional methodologies to solve the problem under consideration here: that of optimising maintenance scheduling and production in processes using decaying catalysts while considering uncertainties in kinetic parameters. In reality, because this is a large scale problem that can contain highly nonlinear equations, obtaining solutions of this problem using conventional methodologies would face significant challenges due to the involvement of mixed-integer optimisation techniques in these methodologies.

The most popular techniques used for optimisation of mixed-integer nonlinear programming problems include the Branch & Bound, Outer Approximation (Duran and Grossmann, 1986; Viswanathan and Grossmann, 1990) and Generalised Benders Decomposition (Geoffrion, 1972) algorithms. However, due to their combinatorial nature, these techniques find it difficult to converge to optimal solutions and require long solution times when used to solve large scale problems. Further, when using mixed-integer techniques, any differential equation present in the problem is approximated as a set of steady state algebraic equations, which are imposed as equality constraints to be fulfilled during the optimisation. Not only does the steady state approximation reduce the solution accuracy, the introduction of additional constraints further increases the problem size and can thereby cause further convergence issues. Due to these drawbacks, mixed-integer techniques face difficulties in obtaining good quality solutions for large scale problems.

A previous work by Adloor et al. (2020) examined the deterministic version of the problem under consideration here, that is, one in which there is no parametric uncertainty involved. In that work it was highlighted how the deterministic problem is itself large scale and how if mixed-integer optimisation techniques were used for solution, the above-mentioned drawbacks of these techniques come into play. If one of the conventional methodologies is used to solve the problem under consideration here, it would involve using mixed-integer techniques to solve a problem of similar or larger size in comparison to the deterministic problem, and so the drawbacks of these techniques would once again be manifested or possibly even be further aggravated.

As mentioned by Li and Ierapetritou (2008b), when using stochastic programming techniques, the number of scenarios to be considered, and so the problem size, increases exponentially with number of uncertain parameters involved and this leads to intractable sizes for large scale problems when such approaches are used with mixed-integer techniques to obtain solutions.

Balasubramanian and Grossmann (2003) report that, when used with fuzzy programming to consider uncertainty, mixed-integer techniques could solve only small scale problems but fail in the case of larger problems due to the intractable sizes encountered. The larger problems could only be solved using meta-heuristic optimisation techniques, which however, cannot provide a theoretical guarantee of the optimality of the solutions obtained.

When parametric programming is used for mixed-integer problems involving uncertainty, the established procedures entail solving a series of parametric and mixed-integer problems (e.g. by Dua and Pistikopoulos (2000), Li and Ierapetritou (2007), Wittmann-Hohlbein and Pistikopoulos (2012)), the latter which is larger in size compared to the deterministic problem. And when using robust optimisation techniques, a robust counterpart of the deterministic problem is formulated (Gorissen et al., 2015), which is comparable in size to that of the latter. Therefore, if the deterministic problem is itself large scale and intractable to solve using mixed-integer techniques, similar difficulties will be experienced by such techniques if used with parametric and robust optimisation methods for optimisation under uncertainty.

Thus, intractable problem sizes, and therefore convergence issues, are likely to be faced when mixed-integer techniques are used with any of the popular preventive methods of handling uncertainty to solve the large scale problem under consideration here. Further, even if solutions can be obtained by any of the conventional methodologies, the practice in mixed-integer techniques, of approximating differential equations as sets of steady state algebraic equations, implies that the solutions cannot be considered accurate.

Hence, it is concluded that conventional methods would not be well suited to solve the problem under consideration here. A methodology is needed that can effectively solve this problem. The contribution of this paper lies in the development of such a methodology: a novel approach that formulates this problem as an optimal control problem. The structure of the optimal control problem formulation is similar to that developed in the previous work by Adloor et al. (2020) which solved the deterministic version of this problem.

This completes Section 1, which constitutes the introductory and literary review part of the paper. The rest of the paper is organised as follows. In Section 2, the optimal control formulation of this problem is developed. Section 3 details the solution methodology and the advantages that this formulation and solution methodology can offer over the conventional methods of solving such problems. In Section 4, the proposed formulation and solution methodology are applied to identify the effects of uncertainties in kinetic parameters on the optimal process operations through different case studies, and the results obtained for each case study are analysed in Section 5. Section 6 contains the conclusions and other notable points.

This paper is an extension of the work of Adloor et al. (2020) and hence, parts of that work are presented in the appendices for reference. Appendix A details a solution methodology developed in that work which forms a part of the solution methodology discussed in Section 3. And Appendix B presents the details of the formulation of an industrial process examined in that work. The case studies formulated in Section 4 are based on a modification of this formulation to include uncertainty in the kinetic parameters. The solution implementation details are mentioned in Appendix C.

2. The optimal control formulation

In this section, an optimal control formulation is presented for the problem of optimising maintenance scheduling and production planning in a process using decaying catalysts, while considering uncertainty in the kinetic parameters of the process model. This formulation is characterised by a set of decision (or control) variables, state variables, a set of Ordinary Differential Equations (ODEs) and constraints, with the uncertainties occurring in the parameters present in the ODEs.

A basic optimal control problem (OCP) is represented by equations (1a) – (1g). The performance index consists of point and continuous indices ϕ, and L, respectively. This performance index is minimised by the selection of controls, w, and the resulting differential state variables, x, when subject to differential equations, h and constraints, c. Equations (1b) – (1c) define an ODE system, given fixed initial and final times, t_0 and t_F, respectively, and initial condition x_0. The controls w comprise binary controls, u, as well as continuous controls, v, which belong to a real permissible set $\mathcal{V}$.

$$\min_{w(t)} W \quad = \quad \phi\left(x(t_F)\right) \; + \int_{t_0}^{t_F} L\left(x(t),\, w(t),\, t\right) \mathrm{d}t \tag{1a}$$

subject to

$$\begin{aligned} \dot{x}(t) = h\left(x(t),\, w(t),\, t\right) \\ \forall t \, \in \, [t_0, t_F] \end{aligned} \tag{1b}$$

$$x\left(t_0\right) = x_0 \tag{1c}$$

$$\begin{aligned} c\left(x(t),\, w(t),\, t\right) \leq \;\; 0 \\ \forall t \, \in \, [t_0, t_F] \end{aligned} \tag{1d}$$

$$w(t) = \left[\left[u(t)\right]^T,\, \left[v(t)\right]^T\right]^T \tag{1e}$$

$$u(t) \, \in \{0, 1\} \tag{1f}$$

$$v(t) \, \in \mathcal{V} \tag{1g}$$

The OCP formulation is applied to the problem under consideration by discretising the whole time horizon of the process into stages, which are of known and fixed lengths. The lengths of different stages can be different. A control parametrisation approach is used wherein the decision variables are discretised and considered piecewise constant across the times corresponding to each stage. That is, the controls u and v, take up the form:

$$u = \left[u^{(1)},\, u^{(2)},\, \ldots,\, u^{(NP)}\right]^T \tag{2a}$$

$$v = \left[v^{(1)},\, v^{(2)},\, \ldots,\, v^{(NP)}\right]^T \tag{2b}$$

where NP is the total number of stages. The control profiles can be discontinuous at the junctions, t_p, between any two consecutive stages, p and $p+1$.

On the other hand, the state variables are maintained in their continuous form, without discretisation, and are determined in each stage from a set of ODEs. This solution methodology is called a "feasible path approach" because the ODEs are solved to a high accuracy, using state-of-the-art integrators, in the right sequential order (Vassiliadis, 1993; Vassiliadis et al., 1994a,b). Junction conditions between any two consecutive periods, p and $p+1$, are used to obtain the solutions of the ODEs in each stage, across the whole time horizon. The general form of these junction conditions is given by equation (3) (Vassiliadis, 1993):

$$\begin{aligned} J\Big(\dot{x}^{(p+1)}\left(t_p^+\right),\, x^{(p+1)}\left(t_p^+\right),\, u^{(p+1)}\left(t_p^+\right),\, v^{(p+1)}\left(t_p^+\right),& \\ \dot{x}^{(p)}\left(t_p^-\right),\, x^{(p)}\left(t_p^-\right),\, u^{(p)}\left(t_p^-\right),\, v^{(p)}\left(t_p^-\right),\, t_p\Big) &= 0 \\ p = 1,\, 2,\, \ldots NP-1 & \end{aligned} \tag{3}$$

The discretisation of the time horizon into multiple stages in this OCP that has integer and continuous decision variables leads to a Multistage Mixed-Integer Optimal Control Problem (MSMIOCP). The basic form of the MSMIOCP is represented by equations (4a) – (4g). The terminology used in equation (4) are similar to the basic OCP formulation in equation (1), with the superscript (p) indicating that they apply to stage p. The additional terms here are the junction conditions, g, analogous to equation (3), that provide the initial conditions for the solution of the ODEs in stage p. An illustration of the MSMIOCP formulation is shown in Figure 1.

$$\min_{u,v} W = \sum_{p=1}^{NP} \left\{ \phi^{(p)} \left(x^{(p)}(t_p),\, u^{(p)},\, v^{(p)},\, t_p \right) + \int_{t_{p-1}}^{t_p} L^{(p)} \left(x^{(p)}(t),\, u^{(p)},\, v^{(p)},\, t \right) \mathrm{d}t \right\} \tag{4a}$$

subject to

$$\begin{gathered} \dot{x}^{(p)}(t) = h^{(p)}(x^{(p)}(t),\, u^{(p)},\, v^{(p)},\, t) \\ t_{p-1} \leq t \leq t_p \\ p = 1, 2, \ldots, NP \end{gathered} \tag{4b}$$

$$x^{(1)}(t_0) = g^{(1)} \left(u^{(1)},\, v^{(1)} \right) \tag{4c}$$

$$\begin{gathered} x^{(p)}(t_{p-1}) = g^{(p)} \left(x^{(p-1)}(t_{p-1}),\, u^{(p)},\, v^{(p)} \right) \\ p = 2,\, 3, \ldots,\, NP \end{gathered} \tag{4d}$$

$$\begin{gathered} c^{(p)} \left(x^{(p)}(t),\, u^{(p)},\, v^{(p)},\, t \right) \leq \; 0 \\ t_{p-1} \leq t \leq t_p \\ p = 1, 2, \ldots, NP \end{gathered} \tag{4e}$$

$$\begin{gathered} u^{(p)} \in \{0, 1\} \\ p = 1,\, 2, \ldots,\, NP \end{gathered} \tag{4f}$$

$$\begin{gathered} v^{(p)} \in \mathcal{V} \\ p = 1,\, 2, \ldots,\, NP \end{gathered} \tag{4g}$$

This MSMIOCP formulation is similar to that developed in a previous

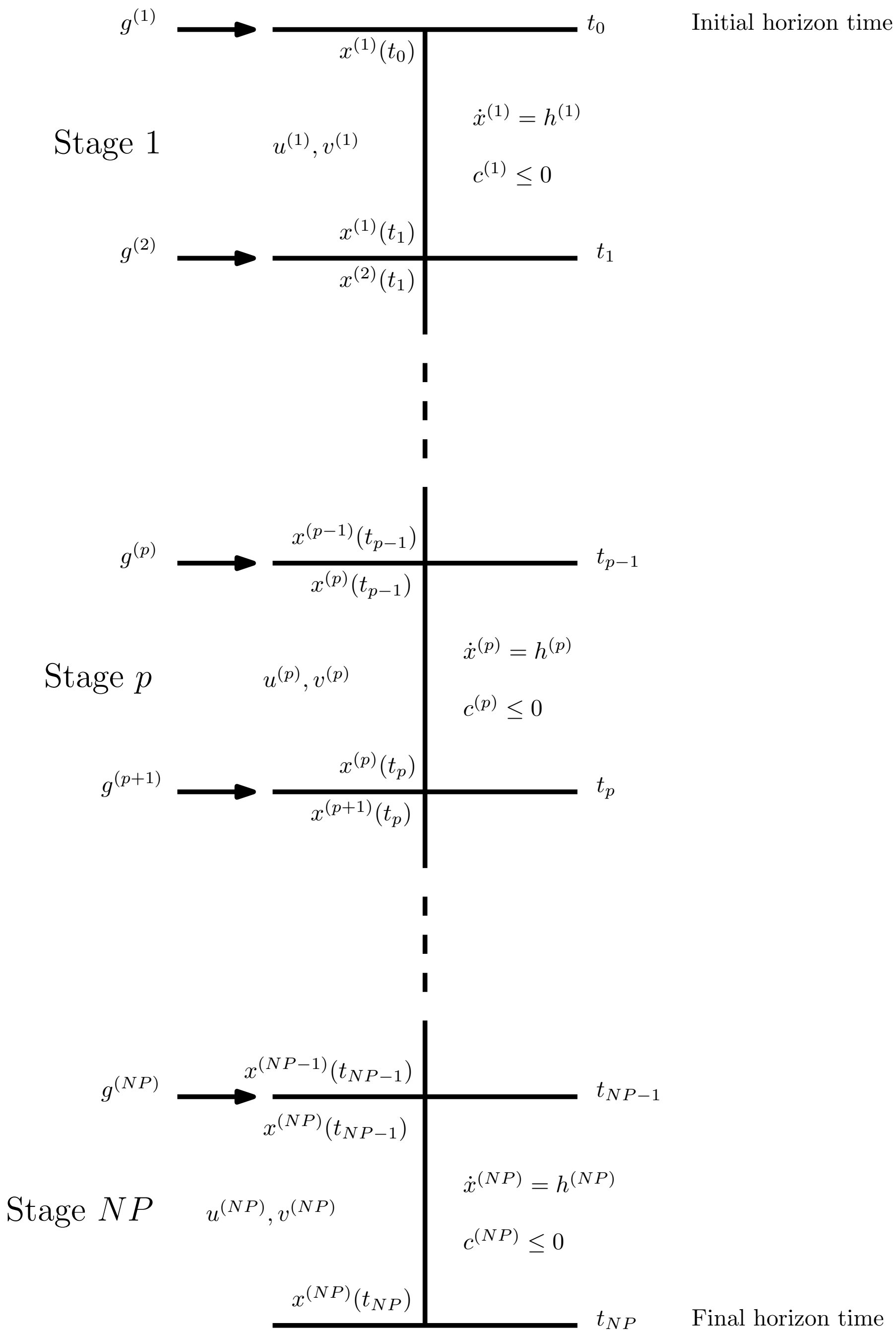

Figure 1: An illustration of the MSMIOCP formulation

work by Adloor et al. (2020), which solved the deterministic version of the problem under consideration here. As in that work, in each stage of the formulation here, a decision of binary nature has to be made on whether the catalyst should continue to be in operation or be replaced, and these variables correspond to the controls, u. Further, the plant operating conditions of flow rate and temperature, and the amount of product sales should also be decided at each stage, which are decisions corresponding to the continuous controls, v.

However, unlike that work, here there is uncertainty regarding the values of the kinetic parameters present in the differential rate equations of the catalyst deactivation and product formation reactions in each stage. Therefore, here a mixed-integer optimisation problem involving parametric uncertainties has to be solved to ensure optimal operation of the process.

As mentioned in Section 1, due to the involvement of mixed-integer optimisation techniques, the conventional methodologies would not be well suited to solving such a formulation. Hence, in the next section, a solution methodology is presented that aims at effectively solving this problem.

3. Problem solution methodology

The solution methodology proposed to solve this problem is comprised of two major parts. In the first part, a novel approach is proposed to consider uncertainties, by developing a stochastic version of the MSMIOCP formulation of Section 2. The second part is to solve this stochastic MSMIOCP formulation as a standard nonlinear optimisation problem using a technique developed in a previous work by Adloor et al. (2020).

In the first part of this methodology, in order to consider parametric uncertainty, a multiple scenario approach is used. That is, multiple scenarios are generated, where in each scenario, each uncertain parameter takes a particular value within a pre-specified range. These scenarios can be generated through any random sampling method.

As mentioned in Section 2, the uncertainties in this problem occur in the parameters present in the ODEs of the MSMIOCP formulation. Thus, for each scenario generated, a new ODE system, comprised of the ODEs, initial and junction conditions, is formed, the parameter values of which correspond to the scenario generated. And the state variables describing each scenario can be determined by the solution of the ODE system corresponding to each scenario. The uncertainty in the problem is represented by the different scenarios: by all the different parameters and state variables values attainable. The aim is to perform the optimisation while ensuring that the uncertainty represented by the different scenarios are accounted for.

A feature of the solution procedure of any OCP is that the integration phase is independent of the optimisation phase. That is, any ordinary differential or differential algebraic equations present have to be integrated completely to obtain values of the state variables, which in turn are used to formulate the objective function and constraints based on which the optimisation can occur. This feature will be exploited here to perform the optimisation under uncertainty.

A new MSMIOCP is formulated wherein the ODE systems corresponding to all scenarios are stacked together. However, while the state variables obtained from the ODE system for each scenario lead to a unique set of constraints and objective function corresponding to that scenario, only the averages of these over all scenarios are used in this MSMIOCP. That is, the decision (or control) variables have to be chosen to optimise only the average of the objective functions over all scenarios while fulfilling only the average of each set of constraints over all scenarios. Thus, this new MSMIOCP is a stochastic version of the formulation presented in equation (4) and is given by equation (5).

In equation (5), W_s is the performance index of the stochastic MSMIOCP and S is the number of scenarios considered. A separate term $\overline{C}^{(p)}$ is introduced to represent the average of the set of constraints over all scenarios in stage p, as shown in equation (5e). The remainder of the terminology used are similar to the MSMIOCP formulation in equation (4) with the only difference being that where subscript z occurs, it represents the variable in scenario z.

$$\begin{aligned} \min_{u,v} W_s \quad &= \quad \frac{1}{S}\left[\sum_{z=1}^{S}\left\{\sum_{p=1}^{NP}\phi_z^{(p)}\left(x_z^{(p)}(t_p),\, u^{(p)},\, v^{(p)},\, t_p\right)\right.\right. \\ &\left.\left. + \int_{t_{p-1}}^{t_p} L_z^{(p)}\left(x_z^{(p)}(t),\, u^{(p)},\, v^{(p)},\, t\right)\,\mathrm{d}t\right\}\right] \end{aligned} \tag{5a}$$

subject to

$$\begin{gathered} \dot{x}_z^{(p)}(t) = h_z^{(p)}(x_z^{(p)}(t),\, u^{(p)},\, v^{(p)},\, t) \\ t_{p-1} \le t \le t_p \\ p = 1, 2, \ldots, NP \\ z = 1, 2, \ldots, S \end{gathered} \tag{5b}$$

$$\begin{gathered} x_z^{(1)}(t_0) = g_z^{(1)}\left(u^{(1)},\, v^{(1)}\right) \\ z = 1, 2, \ldots, S \end{gathered} \tag{5c}$$

$$\begin{gathered} x_z^{(p)}(t_{p-1}) = g_z^{(p)}\left(x_z^{(p-1)}(t_{p-1}),\, u^{(p)},\, v^{(p)}\right) \\ p = 2,\, 3, \ldots,\, NP \\ z = 1, 2, \ldots, S \end{gathered} \tag{5d}$$

$$\overline{C}^{(p)} \leq 0$$

where

$$\overline{C}^{(p)} = \frac{1}{S}\left[\sum_{z=1}^{S} c_z^{(p)}\left(x_z^{(p)}(t),\, u^{(p)},\, v^{(p)},\, t\right)\right] \tag{5e}$$

$$t_{p-1} \leq t \leq t_p$$

$$p = 1, 2, \ldots, NP$$

$$\begin{aligned} u^{(p)} &\in \{0, 1\} \\ p &= 1,\, 2, \ldots,\, NP \end{aligned} \tag{5f}$$

$$\begin{aligned} v^{(p)} &\in \mathcal{V} \\ p &= 1,\, 2, \ldots,\, NP \end{aligned} \tag{5g}$$

In this stochastic MSMIOCP formulation, it is seen how the feature of the integration and optimisation phases being independent of each other is used to advantage: the use of multiple scenarios leads to the size of the ODE system in the integration phase to increase proportionately compared to a single scenario case, but the number of control variables and constraints involved in the optimisation is the same as in a single scenario case. Hence, only a single optimisation problem has to be solved, which has the same number of decision variables and constraints compared to the deterministic problem, but with a larger ODE system compared to the latter.

A schematic describing the underlying principle of this formulation is shown in Figure 2. A similar principle has been used for optimisation under uncertainty in works by Al Ismaili et al. (2019) for scheduling of heat exchanger network cleaning operations and by Kanavalau et al. (2019) in model predictive control for batch process intensification.

This stochastic MSMIOCP formulation is mixed-integer in nature due to the presence of integer and continuous variables. However, as mentioned

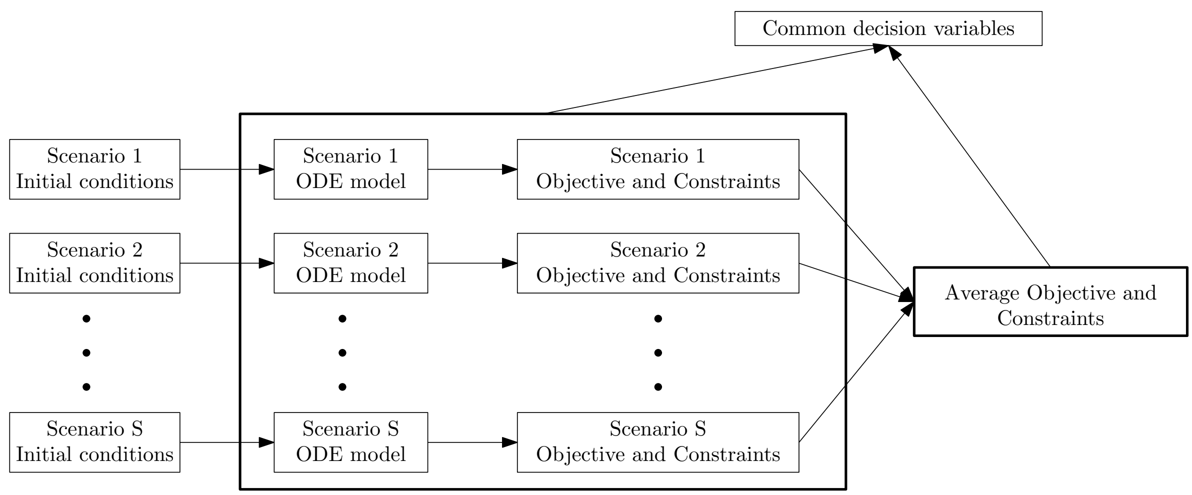

Figure 2: The schematic of the principle of a stochastic optimal control formulation

in Section 1, there are drawbacks to using mixed-integer optimisation techniques. Hence, here a procedure is used that enables solution as a standard nonlinear optimisation problem, without the use of mixed-integer optimisation techniques. This forms the second part of the solution methodology.

This solution procedure, titled Implementation II, was developed in the previous work by Adloor et al. (2020) and the exact details of this procedure are given in Appendix A. Essentially, this procedure enables solution of an MSMIOCP as a standard multistage optimal control problem (MSOCP) while using the feasible path approach to solve ODEs. The binary variables are considered continuous variables in the range $[0, 1]$ and the 0 or 1 values are enforced inherently during the optimisation using a penalty term homotopy technique instead of mixed-integer methods. In the work of Adloor et al. (2020), this procedure was very successful in obtaining optimal solutions for large scale problems, and was able to overcome the drawbacks of mixed-integer optimisation techniques by demonstrating advantages of robustness, reliability and efficiency over those techniques in solving those problems.

In Section 1, it was discussed how due to the involvement of mixed-integer optimisation techniques in the conventional methodologies, these methodologies would not be well suited to solve the large scale problem under consideration in this paper. The solution methodology proposed in this section can provide a number of potential advantages over the conventional methodologies in solving this problem, by overcoming the drawbacks that would be introduced by the use of mixed-integer optimisation techniques in those methodologies. These potential advantages are similar to those demonstrated by the optimal control methodology comprising the procedure of Implementation II in the work of Adloor et al. (2020), and are enumerated as follows:

1. The practice in mixed-integer techniques of approximating differential equations as collections of steady state algebraic equations, often causes the problem to end up containing a very large number of variables and constraints. This can cause difficulties in convergence to optimal solutions when the conventional methodologies are used, especially in the cases of mixed-integer techniques being used with stochastic or fuzzy programming approaches.
   However, the use of the feasible path approach in the proposed methodology implies that the differential equations will be solved by an integrator without creating additional variables or constraints to be considered in the optimisation phase. Therefore, when using the proposed methodology, the number of variables and constraints will be considerably smaller than when any of the conventional methodologies are used. Hence, the methodology is expected to be more robust in converging to solutions in comparison to the conventional methodologies.

2. The feasible path approach employs state-of-the-art integrators which can solve nonlinear differential equations to a high accuracy. On the other hand, the mixed-integer formulations, when used with any of the

existing preventive methods of handling uncertainty, solve such equations by approximations as sets of steady state algebraic equations, and this tends to reduce the accuracy of the solutions. Thus, the solutions obtained by the proposed methodology can be expected to be more reliable than those obtained by the conventional methodologies.

3. By virtue of the penalty term homotopy technique in Implementation II, a weight term in the objective function forces the controls, originally binary but considered continuous in this formulation, to take values of either 0 or 1. Thus, the 0 or 1 values for these controls, which correspond to the catalyst changeover actions in the problem under consideration here, are decided inherently during the optimisation, without using mixed-integer techniques.

   Hence, no additional computational effort will be spent in deciding when to schedule catalyst changeovers, thereby underlining the potential efficiency of this methodology. This feature will enable saving a large amount of computational effort which would be required in the huge number of combinations to be considered when mixed-integer formulations are used with the existing preventive methods of handling uncertainty, especially the stochastic or fuzzy programming approaches.

However, in this formulation, since the number of ODEs scales with the number of scenarios involved, if a large number of scenarios are considered, as would be needed to sufficiently take uncertainty into account, the number of ODEs in the formulation would become very large. The use of the feasible path approach implies considerable computational effort is spent in solving each differential equation to a high accuracy in each iteration of the optimisation, even in those iterations away from the optimal solution. Hence, the computational time is expected to be large for this solution methodology.

While this can be perceived as a drawback of this solution methodology, it is highlighted that the scalability of the formulation can be exploited to reduce computation time. With the advent of parallel computing and high performance computing facilities in today's world, each ODE set or even each differential equation can be simulated entirely on a separate computer. Further, any required gradient evaluations can be parallelised within the computer on which each simulation occurs.

Another limitation is that since this is a non-convex problem, only local optima can be obtained by the proposed methodology. Thus, several runs using different start points have to be performed to identify the global optimum. The high performance and parallel computing facilities would make such a task feasible as well.

The preceding discussion suggests that the proposed solution methodology has the potential to effectively solve the problem under consideration in this paper while overcoming the drawbacks that would be introduced by the use of mixed-integer optimisation techniques in the conventional methodologies of solving this problem. In the next set of sections, the proposed formulation and solution methodology are applied to identify the effects of uncertainties in kinetic parameters on the optimal solutions through different case studies.

4. Case Studies: Problem formulation

It is intended to use case studies to examine the effects of uncertainty in values of the kinetic parameters in the optimisation of the scheduling of changeovers of decaying catalysts in an industrial process in tandem with the planning of its operating conditions and sales to meet seasonal demand. These case studies are derived from a modification of a case study in a previous work by Adloor et al. (2020) to include uncertainty in the kinetic parameters.

The work by Adloor et al. (2020) proposed an optimal control approach to optimise the scheduling of changeovers of decaying catalysts in tandem with the operating conditions and sales to meet seasonal demand. In what was an unrealistic assumption, all parameters values were considered to be known exactly and a deterministic MSMIOCP formulation, of structure similar to that of equation (4), was developed. The MSMIOCP formulation of one of the case studies investigated in that work is given in Appendix B.

In this work, the case study in Appendix B is modified to include uncertainty in the kinetic parameters, and to identify the effect of these uncertainties on the optimal maintenance schedule and production operations, the following case studies are investigated:

Case Study A: Effect of uncertainty in the catalyst deactivation rate constant, Kd

Case Study B: Effect of uncertainty in the pre-exponential factor, Ar, of the product formation reaction

Case Study C: Effect of uncertainty in the activation energy, Ea, of the product formation reaction

Case Study D: Parametric uncertainty study that considers the effect of simultaneous uncertainty in all kinetic parameters and the number of scenarios generated

The procedure that will be used to solve all these case studies, is to first develop an MSMIOCP formulation of this industrial problem, of the structure of equation (4), and then apply the solution methodology proposed in Section 3.

For the MSMIOCP formulation of this industrial problem, the case study presented in Appendix B will be used equivalently, with the exception that either one or all of the kinetic parameters Kd, Ar and Ea are uncertain, depending in the case study. In the following text, the first part of the solution methodology is applied by developing a stochastic formulation of this industrial problem by using this MSMIOCP formulation as basis. In this stochastic MSMIOCP formulation, all kinetic parameters are considered uncertain and hence, it pertains to Case Study D. The stochastic formulations for Case Studies A, B and C are derived from minor modifications of this formulation, and these modifications will be detailed later.

As mentioned in Section 3, this stochastic MSMIOCP formulation incorporates parametric uncertainty by generating multiple scenarios, with each uncertain parameter taking a particular value within a pre-specified range in each scenario. Here, the total number of scenarios generated is given by NS. The kinetic parameters of the catalyst deactivation rate constant, the pre-exponential factor and the activation energy of the product formation reaction generated in scenario $z \in \{1, 2, \ldots, NS\}$ of this formulation are represented by $\widetilde{Kd_z}$, $\widetilde{Ar_z}$ and $\widetilde{Ea_z}$, respectively and these are the counterparts of Kd, Ar and Ea, respectively, in the MSMIOCP formulation.

Following from Section 3, the decision variables in this stochastic formulation remain the same as in a deterministic formulation and so the same terminology as in Appendix B, applies here for the decision variables. The catalyst changeover decision variables, $y(i)$, for each month $i \in \{1, 2, \ldots, NM\}$, corresponds to the binary control u in equation (5f). The decisions of the amount of reactor feed flow rate, $ffr(i, j)$, temperature of operation, $T(i, j)$ and quantity of sales, $sales(i, j)$ for each week, $j \in \{1, 2, 3, 4\}$, of each month $i \in \{1, 2, \ldots, NM\}$, correspond to the continuous control v in equation (5g).

However, as per Section 3, the unique kinetic parameter values in each scenario lead to a corresponding unique set of state variables and their deriving ODE systems, comprised of ODEs, initial conditions and junction conditions. The state variables of catalyst activity, reactant exit concentration, inventory level and cumulative inventory costs attained in scenario $z \in \{1, 2, \ldots, NS\}$, are represented by the symbols $\widetilde{cat\_act}_z$, $\widetilde{cR}_z$, $\widetilde{inl}_z$ and $\widetilde{cum\_inc}_z$, respectively, and these are the counterparts of cat_act, cR, inl and cum_inc, respectively, in the MSMIOCP formulation. The ODE systems for each of these state variables, in each scenario $z \in \{1, 2, \ldots, NS\}$ are presented next. The explanations for their formulation are similar to that of their MSMIOCP counterparts and can be found in Appendix B.

The ODEs for each state variable in each scenario $z \in \{1, 2, \ldots, NS\}$, of the form of equation (5b), are given by equations (6) – (9) and these are the counterparts of ODEs (B.4), (B.7) – (B.9), respectively, in the MSMIOCP formulation. These ODEs are to be solved repeated over a weekly time span, over each week $j \in \{1, 2, 3, 4\}$, of month $i \in \{1, 2, ..., NM\}$ of the time horizon.

$$\frac{\mathrm{d}\left(\widetilde{cat\_act}_z\right)}{\mathrm{d}t} = y(i) \times \left[-\widetilde{Kd}_z \times \widetilde{cat\_act}_z\right] \tag{6}$$

$$\begin{aligned}\frac{\mathrm{d}\left(V \times \widetilde{cR}_z\right)}{\mathrm{d}t} =& ffr(i,j) \times \left(CR0 - \widetilde{cR}_z\right) \\ &- y(i) \times \left[V \times \widetilde{Ar}_z \times exp\left(-\frac{\widetilde{Ea}_z}{R_g \times T\left(i,j\right)}\right) \times \widetilde{cat\_act}_z \times \widetilde{cR}_z\right]\end{aligned} \tag{7}$$

$$\frac{\mathrm{d}\left(\widetilde{inl}_z\right)}{\mathrm{d}t} = y(i) \times \left[V \times \widetilde{Ar}_z \times exp\left(-\frac{\widetilde{Ea}_z}{R_g \times T\left(i,j\right)}\right) \times \widetilde{cat\_act}_z \times \widetilde{cR}_z\right] \tag{8}$$

$$\frac{\mathrm{d}\left(\widetilde{cum\_inc_z}\right)}{\mathrm{d}t} = \widetilde{inl_z} \times icf \tag{9}$$

The initial conditions for week 1 of month 1 for each of the state variables, in each scenario $z \in \{1, 2, \ldots, NS\}$, of the form of equation (5c), are given by equations (10) – (13) and are the counterparts of initial conditions (B.11) – (B.14), respectively, in the MSMIOCP formulation:

$$init\_\widetilde{cat\_act_z}\,(1,1) \;=\; start\_cat\_act \tag{10}$$

$$init\_\widetilde{cR_z}\,(1,1) \;=\; CR0 \tag{11}$$

$$init\_\widetilde{inl_z}\,(1,1) \;=\; 0 \tag{12}$$

$$init\_\widetilde{cum\_inc_z}\,(1,1) \;=\; 0 \tag{13}$$

The junction conditions that link the state variable values between any two consecutive weeks in each scenario $z \in \{1, 2, \ldots, NS\}$, of the form of equation (5d), are given by equations (14) – (17) and these are the counterparts of the junction conditions (B.15) – (B.18), respectively, in the MSMIOCP formulation:

$$\begin{gathered} init\_\widetilde{cat\_act_z}\,(i,\, j+1) \;=\; end\_\widetilde{cat\_act_z}(i,\, j) \\ \forall j = 1, 2, 3 \qquad \forall i = 1, 2, \ldots, NM \end{gathered} \tag{14a}$$

$$\begin{aligned} init\_\widetilde{cat\_act_z}\,(i,\, 1) \;\; &= \left[y(i) \times end\_\widetilde{cat\_act_z}(i-1,\, 4)\right] \\ &\quad + \left[(1 - y(i)) \times start\_cat\_act\right] \end{aligned} \tag{14b}$$

$$\forall i = 2, 3, \ldots, NM$$

$$\begin{gathered} init\_\widetilde{cR_z}\,(i,\, j+1) \;=\; end\_\widetilde{cR_z}(i,\, j) \\ \forall j = 1, 2, 3 \qquad \forall i = 1, 2, \ldots, NM \end{gathered} \tag{15a}$$

$$init\_\widetilde{cR_z}(i,\,1) = \left[y(i) \times end\_\widetilde{cR_z}(i-1,\,4)\right] + \left[(1-y(i)) \times CR0\right] \qquad \forall i = 2,3,\ldots,NM \tag{15b}$$

$$init\_\widetilde{inl_z}\,(i,\,j+1) \;=\; end\_\widetilde{inl_z}(i,\,j) - sales(i,\,j) \qquad \forall j = 1,2,3 \qquad \forall i = 1,2,\ldots,NM \tag{16a}$$

$$init\_\widetilde{inl_z}\,(i,\,1) \;=\; end\_\widetilde{inl_z}(i-1,\,4) - sales\,(i-1,\,4) \qquad \forall i = 2,3,\ldots,NM \tag{16b}$$

$$init\_\widetilde{cum\_inc_z}\,(i,\,j+1) \;=\; end\_\widetilde{cum\_inc_z}(i,\,j) \qquad \forall j = 1,2,3 \qquad \forall i = 1,2,\ldots,NM \tag{17a}$$

$$init\_\widetilde{cum\_inc_z}\,(i,\,1) \;=\; end\_\widetilde{cum\_inc_z}(i-1,\,4) \qquad \forall i = 2,3,\ldots,NM \tag{17b}$$

The constraints in this stochastic formulation, of the form of equation (5e), are formulated on the basis that only the averages of the sets of constraints generated over all scenarios are required to be fulfilled. Among the constraints in the MSMIOCP formulation, given by (B.19) – (B.27) in Appendix B, only constraints (B.26) and (B.27) are influenced by the generation of multiple scenarios. Hence, in this stochastic MSMIOCP formulation, constraints (B.19) – (B.25) apply as in the MSMIOCP formulation, while constraints (B.26) and (B.27) are modified into their stochastic counterparts, given by equations (18) and (19), respectively:

$$\frac{1}{NS}\left[\sum_{z=1}^{NS} end\_\widetilde{cat\_act_z}\,(i,\,4)\right] \geq \;\; min\_cat\_act \tag{18}$$

$$\frac{1}{NS}\left[\sum_{z=1}^{NS} end\_\widetilde{inl_z}(i,\,j)\right] - sales(i,j) \geq \;\; 0 \tag{19}$$

And finally, the objective function of the stochastic formulation, of the form of equation (5a), is formulated. It is highlighted that among the components of the objective function in the MSMIOCP formulation, given by equations (B.28) – (B.37), only the Total Inventory Cost (TIC), given by equation (B.30), is influenced by the generation of multiple scenarios and its counterpart in the stochastic formulation is given by equation (20):

$$\begin{aligned} \widetilde{TIC}_z \;&=\; end\_cum\_\widetilde{inc}_z(NM,\,4) \\ &\forall z = 1, 2, \ldots, NS \end{aligned} \tag{20}$$

As per the proposed solution methodology, only the average of the net inventory costs over all scenarios will be included in the objective function of the stochastic formulation. The remaining components of this objective function are the same as those given by (B.28), (B.29) and (B.31) – (B.37) in the MSMIOCP formulation, as these are not influenced by the generation of multiple scenarios. Thus, the objective function in this stochastic formulation, which is the counterpart of (B.38) in the MSMIOCP formulation, is given by equation (21):

$$\min NC_s = -GRS + \left[\frac{1}{NS}\left(\sum_{z=1}^{NS} \widetilde{TIC}_z\right)\right] + TCCC + NPUD + TFC \tag{21}$$

where GRS is the Gross Revenue from Sales, $TCCC$ is the Total Cost of Catalyst Changeovers, $NPUD$ is the Net Penalty for Unmet Demand, TFC is the Total Flow Cost and NC_s is the Net Cost in this stochastic formulation.

This concludes the formulation of the stochastic MSMIOCP for Case Study D, wherein all kinetic parameters are considered uncertain. The stochastic MSMIOCP formulation to be used for Case Study A is largely similar to that of Case Study D with the exception that because Kd is the only uncertain parameter involved, the pre-exponential factor and activation energy values in the formulation are fixed to their deterministic values of $\overline{Ar}$ and $\overline{Ea}$, respectively, which are assumed to be known. That is, the stochastic

MSMIOCP formulation of Case Study A is a special case of Case Study D, wherein $\widetilde{Ar_z} = \overline{Ar}, \forall z \in \{1, 2, \ldots, NS\}$ and $\widetilde{Ea_z} = \overline{Ea}, \forall z \in \{1, 2, \ldots, NS\}$.

Similarly, in Case study B where Ar is the only uncertain parameter, the stochastic MSMIOCP formulation is a special case of Case Study D, wherein $\widetilde{Kd_z} = \overline{Kd}, \forall z \in \{1, 2, \ldots, NS\}$ and $\widetilde{Ea_z} = \overline{Ea}, \forall z \in \{1, 2, \ldots, NS\}$, where $\overline{Kd}$, is the known, deterministic value of the catalyst deactivation rate constant. And, in Case study C where Ea is the only uncertain parameter, the stochastic MSMIOCP formulation is a special case of Case Study D, wherein $\widetilde{Kd_z} = \overline{Kd}, \forall z \in \{1, 2, \ldots, NS\}$ and $\widetilde{Ar_z} = \overline{Ar}, \forall z \in \{1, 2, \ldots, NS\}$.

The impact of parametric uncertainty in all case studies is analysed by solving sub-problems within each case study. That is, the results of all sub-problems of the case study together represent the impact of the considered parametric uncertainty in that case study. Depending on the case study, the sub-problems differ either in the range of values considered for the uncertain parameter or the number of scenarios. The details of the sub-problems investigated in each case study follow next.

In both, Case Study A and Case Study B, wherein Kd and Ar are the uncertain parameters, respectively, three sub-problems are examined, that consider values for Kd and Ar in the ranges of 10%, 20% and 30% relative standard deviations (RSDs) around the means assumed to be $\overline{Kd}$ and $\overline{Ar}$, respectively. In each of these sub-problems, $NS = 20$ scenarios are sampled from the respective ranges.

In Case Study C, wherein Ea is the uncertain parameter, three sub-problems are again examined, but because Ea appears within an exponential function in the model, smaller ranges of 5%, 7.5% and 10% RSDs around the mean assumed to be $\overline{Ea}$, are considered. Once again, in each sub-problem,

$NS = 20$ scenarios are sampled from the respective ranges.

And in the parametric uncertainty study of Case Study D, five sub-problems are examined that consider NS values of 5, 10, 15, 20 and 25. For each of these sub-problems, the respective number of scenarios are sampled from only one range of values for each uncertain parameter: 10% RSD around the mean, $\overline{Kd}$, for Kd, 10% RSD around the mean, $\overline{Ar}$, for Ar and 5% RSD around the mean, $\overline{Ea}$, for Ea.

The stochastic MSMIOCP formulated in each sub-problem of each case study is solved using the second part of the proposed solution methodology. That is, each is solved as a series of standard MSOCPs using the feasible path approach, by applying the procedure of Implementation II, as given in Appendix A, and solving a set of problems of the following form:

$$\begin{aligned} G_k : \min \ & \left[NC_s + M_k \sum_{i=1}^{NM} y(i) \left[1 - y(i)\right] \right] \\ & k = 1, 2, 3 \ldots \end{aligned} \tag{22}$$

In each problem, G_k ($k = 1, 2, 3 \ldots$), of the above series, the appropriate ODEs, initial conditions, junction conditions and constraints apply, depending on the case study. As per this procedure, if in the solution of G_k, the condition, $y(i) \in \{0, 1\}, i = 1, 2, \ldots NM$, does not apply, then problem G_{k+1} is solved using the solution of G_k as initial guesses, with weight $M_{k+1} > M_k$.

Details of the parameters that apply for all case studies, the size of the sub-problems for all case studies, and the implementation on Python are given in Appendix C. It is noted that in all sub-problems of all case studies, the initial guesses for the decision variables in the first problem (major iteration) of the series ($k = 1$) in the optimisation were set to their respective upper bounds. And for the choice of parameters used in this article, the weight term in equation (22) is increased as per the arithmetic progression in equation (23):

$$\begin{aligned} M_{k+1} &= (2 \times M_k) + \left(5 \times 10^7\right) \\ M_1 &= 0 \\ k &= 1, 2, 3 \ldots \end{aligned} \tag{23}$$

In the next section, the results obtained for all sub-problems of all case studies are discussed.

5. Results and discussions

It was found that the proposed solution methodology faced no difficulties in obtaining solutions for any sub-problem in any of the case studies, regardless of the ranges of the uncertain parameters considered or number of scenarios involved. In each sub-problem, the ODEs were solved to the specified integration tolerances and the optimisation converged to within the stipulated tolerances, thereby underlining the high quality of solutions obtained.

In each sub-problem, the variations of the decision and state variables over the time horizon were very similar to those obtained in the deterministic (single scenario) study done in Adloor et al. (2020). Hence, these are not discussed here. The reader is referred to the work by Adloor et al. (2020) for a presentation and explanation of the trends of these variables over the time horizon.

The major impacts of parametric uncertainties were seen in the values of objective functions and the time and frequency of catalyst replacements. These properties showed variations between different sub-problem within the same case study as well as in comparison to a deterministic (single scenario) optimisation run performed using the same initial points.

Table 1: Deterministic run solution details

Property	**Value**
Profit (Million $)	447.139
Number of catalyst replacements	4
Months of catalyst replacements	7, 14, 19, 26
Number of major iterations	2
Solution time (seconds)	9183

The deterministic (single scenario) case was run using the values of $\overline{Kd}$, $\overline{Ar}$ and $\overline{Ea}$ for the catalyst deactivation rate constant, pre-exponential factor and activation energy for the product formation reaction, respectively. Details of the solution obtained from this deterministic run, using the same initial points as in all case studies, are given in Table 1. It is noted that the value of "Profit" in Table 1 is equivalent to the value, in the optimal solution, of $-NC$, where NC is given by equation (B.38).

The properties of the results of the sub-problems of the four case studies, analogous to the properties of the deterministic solution in Table 1, are given in Tables 2 – 5. It is noted that the value of "Mean profit over all scenarios" in these tables is equivalent to the value, in the optimal solution, of $-NC_s$, where NC_s is the net costs in the examined sub-problem of the case study, of the form of equation (21). The effects of uncertainty considered in each case study will be analysed by making a comparison between the results of the sub-problems of the case study, as well as comparing the results of these sub-problems with that of the deterministic run.

5.1. Case Study A

Details regarding the solutions obtained from the sub-problems investigated in this case study are given in Table 2 and Figure 3. As can be seen in

Table 2: Case Study A solution details

Property	**%RSD about $\overline{Kd}$**		
	10	**20**	**30**
Mean profit over all scenarios (Million $)	418.832	419.640	420.685
Maximum profit over all scenarios (Million $)	418.905	419.785	420.901
Minimum profit over all scenarios (Million $)	418.760	419.496	420.427
Profit RSD (%)	0.0107	0.0214	0.0321
Number of catalyst replacements	3	3	3
Months of catalyst replacements	7, 19, 26	7, 19, 26	7, 19, 26
Number of major iterations	4	4	4
Solution time (seconds)	703187	811814	1049004

Table 3: Case Study B solution details

Property	**%RSD about $\overline{Ar}$**		
	10	**20**	**30**
Mean profit over all scenarios (Million $)	447.451	441.436	439.689
Maximum profit over all scenarios (Million $)	447.772	442.081	440.667
Minimum profit over all scenarios (Million $)	447.123	440.785	438.715
Profit RSD (%)	0.0452	0.09145	0.1383
Number of catalyst replacements	4	4	4
Months of catalyst replacements	7, 13, 19, 26	7, 12, 19, 26	7, 13, 19, 26
Number of major iterations	2	2	2
Solution time (seconds)	825814	754913	488749

Table 4: Case Study C solution details

Property	%RSD about $\overline{Ea}$		
	5	**7.5**	**10**
Mean profit over all scenarios (Million $)	426.323	465.965	443.435
Maximum profit over all scenarios (Million $)	426.884	466.816	444.523
Minimum profit over all scenarios (Million $)	425.740	465.044	442.213
Profit RSD (%)	0.0837	0.1187	0.1628
Number of catalyst replacements	3	4	3
Months of catalyst replacements	7, 19, 26	7, 13, 19, 26	7, 19, 26
Number of major iterations	4	2	4
Solution time (seconds)	934872	747505	802522

Table 5: Case Study D solution details

Property	Number of scenarios				
	5	**10**	**15**	**20**	**25**
Mean profit over all scenarios (Million $)	458.362	435.290	423.175	425.849	459.550
Maximum profit over all scenarios (Million $)	459.001	435.774	423.901	426.606	460.317
Minimum profit over all scenarios (Million $)	457.731	434.471	422.448	425.102	458.796
Profit RSD (%)	0.1172	0.0990	0.1046	0.1010	0.1015
Number of catalyst replacements	3	4	3	3	4
Months of catalyst replacements	7, 19, 26	7, 13, 19, 26	7, 19, 26	7, 15, 22	7, 13, 19, 26
Number of major iterations	4	2	4	6	2
Solution time (seconds)	95150	308784	1060280	1367039	858033

Table 2, the inclusion of uncertainty in Kd introduces significant differences in comparison to the deterministic solution presented in Table 1.

The expected (mean) profits in the sub-problems of 10%, 20% and 30% RSDs about $\overline{Kd}$ show a considerable decrease of about 29, 28 and 27 million dollars, respectively, from the deterministic solution. It is noted that while the expected profits increase with an expansion in the range of values considered, the increase between sub-problems is relatively small, showing an increase of about 2 million dollars for an expansion in range from 10% RSD to 30% RSD. This suggests that while consideration of uncertainty in Kd does have an impact on the profits of the process, the sensitivity of profits to further change in values of Kd is relatively less. The low sensitivity to change in Kd is also indicated in the small values of the RSDs of the profits generated over all scenarios for all sub-problems.

The RSD values increase as the range of values considered in the sub-problems increases, which is natural. This is also reflected in the increasing difference between the maximum and minimum profits generated over all scenarios as the range of values considered in the sub-problems increases.

It is highlighted that the RSDs of the profits generated over all scenarios are of small magnitudes in all case studies. This can be attributed to the fact that it is only the inventory costs that are impacted by the generation of multiple scenarios and as mentioned in Adloor et al. (2020), these costs form the smallest proportion of the total expenses. However, different magnitudes are observed in different case studies, which suggests different levels of sensitivity of the profits to the change in values of different parameters.

Figure 3 provides an insight into the correlation between the profit and the value of Kd over all scenarios, for each sub-problem. Within all sub-

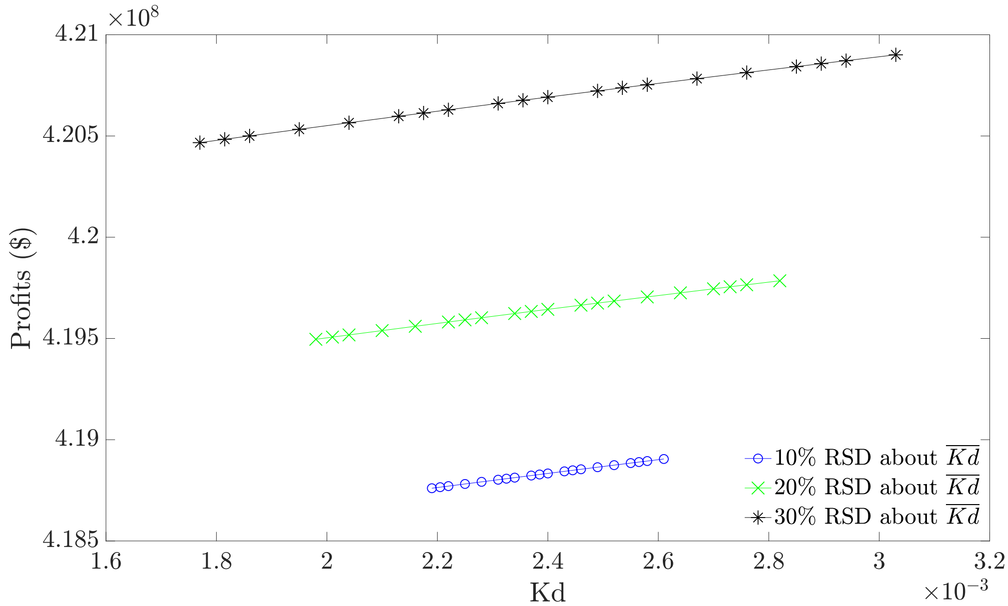

Figure 3: The correlation between value of Kd and profit over all scenarios for the three sub-problems

problems, the profits seem to increase in a linear manner with the increase in value of Kd. This does not mean a generalisation that a higher value of Kd always leads to higher profit. It only implies that for a set of optimal decisions obtained in a particular sub-problem considering a set of scenarios, the nature of equations in the process model is such that the scenario containing a higher value of Kd attains a larger profit.

The number of catalyst replacements and the months in which they occur are the same for all sub-problems in this case study, indicating that these properties are not sensitive to a change in the range of uncertainty for Kd. But the number of catalyst replacements occurring in all of these sub-problems is 3, which is one less than in the deterministic case. However, the months in which these 3 catalyst replacements occur, are the same as the months of 3 of the 4 catalyst replacements in the deterministic case.

Thus, compared to the deterministic case, the inclusion of uncertainty in Kd causes a change in the number of catalyst replacements, but does not cause a variation in the preferred months of catalyst replacement.

The presence of uncertainty in Kd also causes the penalty term homotopy technique in the procedure of Implementation II to operate differently compared to in the deterministic study. Each sub-problem here requires 4 major iterations, or 4 problems of the series given by equation (22) to be solved, to ensure binary values for the catalyst changeover controls. This is different from the deterministic study that required only 2 such major iterations.

The use of several different scenarios to consider parametric uncertainty causes the size of the ODE system to be solved in each of these sub-problems to become several times larger than that of the deterministic study (Table C.8). This causes the solution time for each of these sub-problems to be much larger than that of the deterministic study.

5.2. Case Study B

Details of the solutions obtained from the sub-problems investigated in Case Study B are given in Table 3 and Figure 4. It is seen that the inclusion of uncertainty in Ar also introduces differences in comparison to the deterministic solution.

Compared to the profit in the deterministic solution, the expected profit for the sub-problem of 10% RSD about $\overline{Ar}$ showed a relatively small difference of about 0.3 million dollars, but larger differences of about 6 and 8 million dollars are seen for the sub-problems of 20% and 30% RSD about $\overline{Ar}$, respectively. This suggests that uncertainty in Ar can cause significant differences from the deterministic profit only when larger ranges of uncertainty are considered. Further, the differences from the deterministic solution are less than what was seen for similar ranges of uncertainty for Kd in Case Study A.

This indicates that uncertainty in Ar has a smaller impact on the profits of the process compared to uncertainty in Kd. Another difference from Case Study A is that the expected profits decrease as the range of uncertainty for Ar increases, whereas an opposite trend was seen for uncertainty in Kd.

On the other hand, as the range of uncertainty in Ar is changed, the change in the value of expected profits, the RSDs of the profits generated over all scenarios, as well as the difference between maximum and minimum profits, are larger in comparison to those seen for a similar change of range in Kd in Case Study A. This suggests that the profits are more sensitive to a change in value of Ar compared to a change in value of Kd.

As in Case Study A, a natural increase occurs in the RSDs of the profits generated over all scenarios and the difference between maximum and minimum profits, as the range of uncertainty is increased in this case study.

An insight into the correlation between the profit and the value of Ar over all scenarios for each sub-problem is provided in Figure 4. Within all sub-problems, the profits seem to increase with an increase in Ar value, but unlike in Case Study A, this increase is not linear. Once again, it is stressed that a higher Ar value in a scenario leading to a higher profit in that scenario in each sub-problem, arises from the nature of the process model equations for a fixed set of optimal decisions and is not a trend that can be generalised.

The number of catalyst replacements for all sub-problems in this case study is the same and is equal to in the deterministic study, thereby suggesting that this property is not affected by the inclusion of uncertainty in Ar.

However, on observing the months in which these replacements occur, the timing of the second catalyst replacement appears to vary, by occurring in

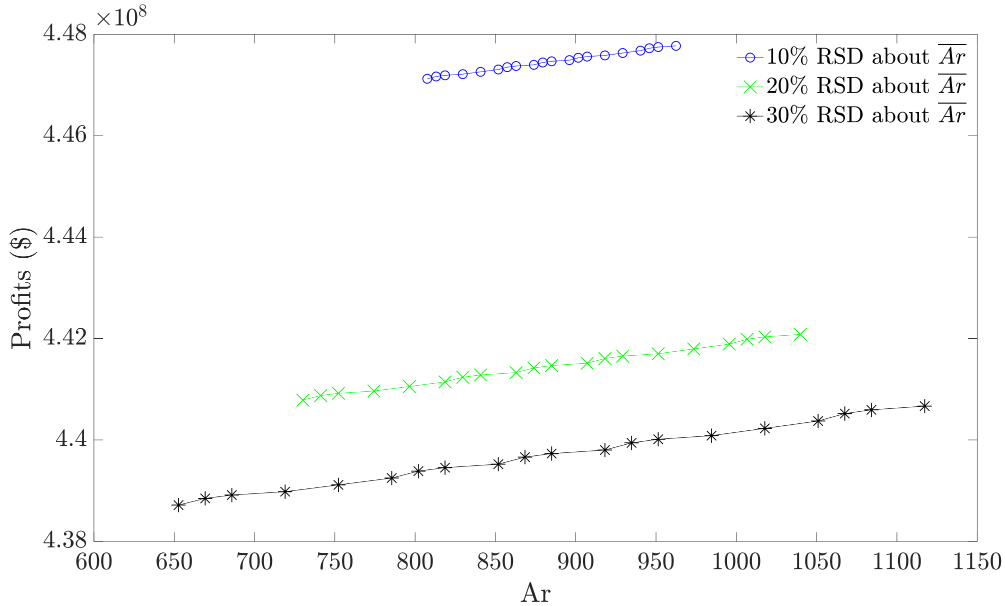

Figure 4: The correlation between value of Ar and profit over all scenarios for the three sub-problems

the 13$^{\text{th}}$ month in the sub-problems of 10% and 30% RSD about $\overline{Ar}$ and in the 12$^{\text{th}}$ month in the sub-problem of 20% RSD about $\overline{Ar}$, in comparison to the 14$^{\text{th}}$ month in the deterministic study. The months of all other catalyst replacements (7, 19 and 26) in all sub-problems are the same as in the deterministic study.

Thus, the observation is that even in the presence of uncertainty in Ar, majority of the catalyst replacements occur at the same time as in the deterministic study, and in the minority of situations when the timing is different, it is within one or two months of the time suggested in the deterministic study. This suggests that while the timing of catalyst replacements is impacted by the uncertainty in Ar, the effects are not drastic in the sense that the timing is only less sensitive to the uncertainty. It is also worth noting that majority of the months of catalyst replacements here overlap with the times suggested in the sub-problems of Case Study A.

As in the deterministic study, all sub-problems in this case study require two major iterations of the penalty term homotopy technique for the catalyst changeover controls to attain binary values. However, due to the large ODE system (Table C.8), the solution times for all these sub-problems are several times larger than that of the deterministic solution.

5.3. Case Study C

Details of the solutions obtained from the sub-problems investigated in Case Study C are given in Table 4 and Figure 5. The occurrence of the uncertain parameter, Ea, in an exponential term, causes the solutions of the sub-problems in this case study to be significantly different from the deterministic study, even while considering smaller ranges of uncertainty in comparison to the previous case studies.

As seen in Table 4, the expected profits for the sub-problems of 5%, 7.5% and 10% RSD about $\overline{Ea}$ were lower by approximately 21 million dollars, higher by approximately 18 million dollars and lower by approximately 4 million dollars respectively, in comparison to the profit of the deterministic solution. Thus, it can be concluded that uncertainty in Ea has a significant effect on the expected profit. However, the wide variation in profit values between sub-problems and the lack of clearly increasing or decreasing trends makes it difficult to compare the effect on the expected profit of uncertainty in Ea with that of the other parameters in the previous case studies.

As in the previous case studies, the RSDs of the profits generated over all scenarios, as well as the difference between maximum and minimum profits in a sub-problem, increase as the range of uncertainty for Ea increases. However, the profit RSD values are comparable to or even larger than those of the parameters in the previous case studies even though ranges of uncertainty

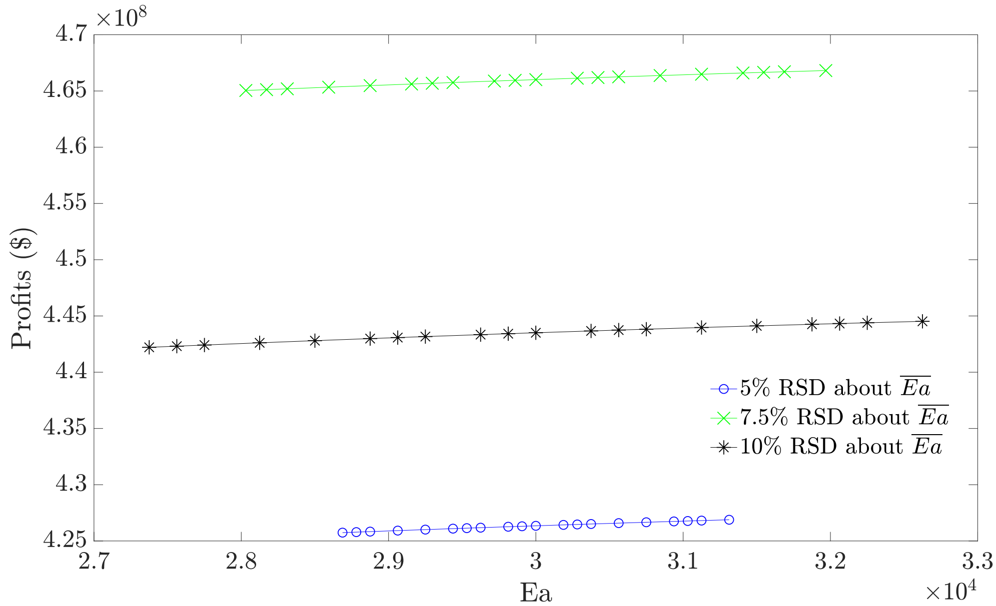

Figure 5: The correlation between value of Ea and profit over all scenarios for the three sub-problems

used for Ea are smaller than those of the parameters in those case studies. This suggests that the profit values are more sensitive to a change in value of Ea compared to a change in value of Ar or Kd. This can be attributed to the occurrence of Ea within an exponential term in the process model against the linear occurrences of Ar and Kd.

The correlation between the profit and the value of Ea over all scenarios for each sub-problem is given in Figure 5. Within all sub-problems, the profits seem to increase with an increase in Ea value in a linear manner. Once again, this is not a trend that can be generalised due to reasons similar to those mentioned in the explanations of the analogous figures (Figures 3 and 4) in the previous case studies.

The number of catalyst replacements in the sub-problem of 7.5% RSD about $\overline{Ea}$ is 4, which is the same as in the deterministic study. But this number drops to 3 in the sub-problems of 5% and 10% RSD about $\overline{Ea}$. This suggests that this property is susceptible to change with varying ranges of uncertainty in Ea.

While the number of catalyst replacements in the sub-problem of 7.5% RSD about $\overline{Ea}$ is the same as in the deterministic study, the second catalyst replacement in this sub-problem occurs in the 13$^{\text{th}}$ month, in comparison to the 14$^{\text{th}}$ month in the deterministic study. The months of the other 3 catalyst replacements (7, 19 and 26) in the sub-problem are the same as in the deterministic study and in fact, these overlap with the months of the 3 catalyst replacements in the sub-problems of 5% and 10% RSD about $\overline{Ea}$. Thus, even in presence of uncertainty in Ea, the catalyst replacements occur mostly at the same time as in the deterministic study or within one month of the time suggested in the latter, in the minority of cases. This indicates that while the timing of catalyst replacements is impacted by the uncertainty in Ea, the sensitivity to uncertainty in Ea is small. The reporting of similar observations in other case studies suggests that the timing of catalyst replacement is less sensitive to the presence of parametric uncertainty.

While the number of major iterations in the penalty term homotopy technique is 2 in the deterministic study and the sub-problem of 7.5% RSD about $\overline{Ea}$, it is 4 in the sub-problems of 5% and 10% RSD about $\overline{Ea}$. As in the previous case studies, due to the large ODE system (Table C.8), the solution times for all these sub-problems are several times larger than that of the deterministic solution.

5.4. Case Study D

Table 5 provides details of the solutions of the sub-problems examined in Case Study D, that considered the effect of simultaneous uncertainty in parameters Kd, Ar and Ea while generating different number of scenarios.

It is noted that the scenarios for each parameter in each sub-problem were generated independently of each other. For example, in the 10 scenario sub-problem, the 10 samples for each parameter were generated exclusively for this sub-problem and not by adding 5 samples to those of the 5 scenario sub-problem.

As is seen in Table 5, the expected profits show significant variations between sub-problems, as well as in comparison to the profit in the deterministic study. The expected profits for the 5, 10, 15, 20 and 25 scenario sub-problems show an increase of about 11 million dollars, a decrease of about 12 million dollars, a decrease of about 24 million dollars, a decrease of about 22 million dollars and an increase of about 12 million dollars, respectively, from the profit in the deterministic study.

The difference between the maximum and minimum profit over all scenarios in each sub-problem shows a gradual increase as the number of scenarios considered in the sub-problem increases. The RSDs of the profit values over all scenarios show slight variations between sub-problems but are mostly around the value of about 0.1%.

The number of catalyst replacements also shows variations between sub-problems: while 4 replacements, the same as in the deterministic study, occur in the sub-problems of 10 and 25 scenarios, only 3 replacements occur in the sub-problems of 5, 15 and 20 scenarios.

While the number of catalyst replacements in the 10 and 25 scenario sub-problems are the same as in the deterministic study, the second catalyst replacement in these sub-problems occurs in the 13$^{\text{th}}$ month, in comparison to the 14$^{\text{th}}$ month in the deterministic study. The months of the other 3 catalyst replacements (7, 19 and 26) in these sub-problems are the same as in the deterministic study and in fact, these overlap with the months of the 3 catalyst replacements in the sub-problems of 5 and 15 scenarios. In the 20 scenario sub-problem, while the timing of the first catalyst replacement (7^{th} month) is consistent with that of the deterministic study and all other sub-problems, the same does not hold for the timings of the second (15^{th} month) and third (22^{nd} month) replacements. This anomaly in the 20 scenario sub-problem could be because a unique local optimum is attained.

However, apart from a few anomalous cases in the 20 scenario sub-problem, the observation is that the timings of catalyst replacements in all sub-problems are mostly the same as in the deterministic study, or within a month of the timing in the latter in the minority of situations. This suggests that the sensitivity of the timing of catalyst replacements to the simultaneous inclusion of uncertainty in all parameters as well as different number of scenarios is small, but not nil. This observation reinforces the suggestions made in the previous sub-sections that the timing of catalyst replacements is less sensitive to the presence of parametric uncertainty.

The number of major iterations in Implementation II also varies between sub-problems. The sub-problems of 10 and 25 scenarios require 2 such iterations, as in the deterministic study, but the sub-problems of 5 and 15 scenarios require 4 such iterations and the 20 scenario sub-problem requires 6 such iterations.

The solution times for all sub-problems are several times larger than in the deterministic study, owing to their larger ODE systems compared to the latter (Table C.8). The 5 scenario sub-problem has the smallest solution time among all sub-problems, followed by the 10 scenario sub-problem, and this follows from the size of their respective ODE systems. It may seem counter-intuitive that the solution time for the 25 scenario sub-problem is smaller than those of the 15 and 20 scenario sub-problems, despite the larger size of the ODE system in the former. This is because a greater number of major iterations are needed for the 15 and 20 scenario sub-problems (4 and 6, respectively) compared to the 25 scenario sub-problem (which required only 2).

Thus, it is seen that the solutions of all sub-problems show variations from the deterministic solution and this is an indication of the significant effects that the inclusion of uncertainty in all parameters simultaneously can produce. But there are also variations between the solutions of the sub-problems, each which considered a different number of scenarios, even though all considered the same range of uncertainty for each uncertain parameter.

The number of major iterations and the solution times for the different sub-problems can be expected to be different, due to the different sizes of the ODE systems involved in each sub-problem. However, the variations in the RSDs of the profits over all scenarios, the number of catalyst replacements, the months of catalyst replacements and especially the large differences in the obtained profit values between sub-problems suggest that an insufficient number of scenarios have been considered to solve this problem. That is, a much larger number of scenarios have to be considered in order to identify the optimal schedule of catalyst replacements and production plan under the given range of uncertainty for each parameter.

5.5. General discussion of results

In this sub-section, a comparative discussion of the results obtained in all case studies is carried out and some conclusions are drawn.

With regard to the expected profit of the process, a comparison of the results of the sub-problems of Case Studies A and B indicate that uncertainty in Ar has a smaller impact compared to uncertainty in Kd. Another notable trend is that the expected profits decrease as the range of uncertainty for Ar

increases, but increase for an increase in range of uncertainty for Kd.

The results of the sub-problems of Case Study C indicate that uncertainty in Ea has a significant impact on the expected profit of the process. However, with increasing range of uncertainty in Ea, there is no pattern in the obtained values of the expected profit, in terms of a variation from the deterministic profit or an increasing or decreasing trend. Hence, no clear comparisons could be drawn between the impact on the expected profits of uncertainty in Ea and uncertainty in Kd or Ar.

On the other hand, a comparison of the RSDs of the profits over all scenarios indicates that the profits of the process are most sensitive to a change in value of Ea, the next highest sensitivity is to a change in value of Ar and the lowest sensitivity is to a change in value of Kd. The highest sensitivity to a change in Ea could be attributed to the occurrence of Ea in an exponential term in the process model, against the linear occurrences of Ar and Kd.

However, in the results of the sub-problems of Case Study D, which considered different number of scenarios, although the RSDs of the profits over all scenarios are all around the value of about 0.1%, the expected profits vary widely between the sub-problems, even though all considered the same range of uncertainty for each uncertain parameter. This indicates that an insufficient number of scenarios were being considered to solve this problem.

To obtain the actual solution of this problem, a much larger number of scenarios need to be considered. The number should be large enough, such that a further increase beyond this number would cause negligible variations in the solutions. However, the computational power required to consider such a large number of scenarios is currently not available to the authors and so, this has not been carried out in this article.

The conclusion from Case Study D, that a much larger number of scenarios is needed to solve this problem, throws a question on the inferences drawn from the solutions of Case Studies A, B and C, as these case studies considered only 20 scenarios, which is certainly not a large number. Therefore, the apparent observations such as the profits being least sensitive to change in Kd, or uncertainty in Ar having a smaller impact on expected profit compared to uncertainty in Kd, cannot be concluded to be true unless the same are observed while considering the required larger number of scenarios.

However, with regard to the the number and timing of catalyst replacements, the results obtained suggest that parametric uncertainty has a small impact. In the results of the sub-problems of all case studies, the optimal number of replacements is either 3 or 4, thus showing small or no variation from the deterministic solution that has 4 replacements. Further, the months of replacements are mostly similar or within one or two months of the times in the deterministic solution, apart from in the 20 scenario sub-problem of Case Study D which can be considered an anomalous result.

This observation suggests that, just by knowing the deterministic solution, the operator of the process can obtain good estimates of the optimal number and timing of catalyst replacements, in the presence of parametric uncertainty. However the fact remains that variations, though small, are seen in these properties between the results of the different number of scenarios considered in Case Study D. The consideration of the required larger number of scenarios can enable obtaining exact values, rather than estimates, of the optimal values of these properties in the presence of parametric uncertainty.

And finally, it is highlighted that only one set of initial guesses was used for the optimisation in all sub-problems of all case studies. As the problem here is non-convex, the solution obtained for each sub-problem is only a local optimum. In order to find the global optimum in each of these problems, the best solution out of several optimisation runs, each carried out using different initial guesses, needs to be identified. This would require a huge amount of computational effort and hence, has not been carried out in this article.

Thus, the results of the different case studies obtained in this article can be said to provide useful insights into the effects of parametric uncertainty in this problem while demonstrating the application of the proposed solution methodology. But these results cannot be concluded as the actual solutions of these case studies. In order to fully identify the effect of each uncertain parameter in Case Studies A, B and C, the sub-problems in these case studies need to be solved while considering a large number of scenarios and by identifying the global optimum from a set of solutions obtained from several different initial guesses. Similarly, the global optimum of the parametric uncertainty problem in Case Study D can be identified from a set of solutions obtained from several different initial guesses, while considering a large number of scenarios for each uncertain parameter.

The advantage of the stochastic formulation in the proposed solution methodology is that only the size of the ODE system increases as the number of scenarios considered increases and the number of decision variables and constraints remain the same as in the deterministic case, regardless of the number of scenarios involved. This property has prevented an explosion in problem size and facilitated convergence to high quality solutions, within the stipulated tolerances, for all case studies considered. Thus, the proposed solution methodology would face no difficulties in obtaining the global optimum of the aforementioned case studies by considering the required number of large scenarios and the several different initial guesses, provided the required computational power is available. The use of high performance computing and parallel computing facilities would make such a task feasible.

6. Conclusions and further discussions

In conclusion, the contribution of this paper is the development of a novel approach that is capable of identifying the optimal maintenance schedule and production plan for an industrial process using decaying catalysts while considering uncertainties in the kinetic parameters of the underlying process model. The novelty of the approach lies in the formulation of this problem as a multistage mixed-integer optimal control problem (MSMIOCP) which is solved using a unique two-part solution methodology. This approach can provide valuable insights into the individual as well as collective effects of uncertainties on the optimal operations. Further, it can also offer a number of potential advantages over the conventional methods of solving problems of this category, by overcoming the drawbacks introduced by the use of mixed-integer optimisation techniques in those methods.

Further discussions can be drawn regarding the proposed methodology. In the multiple scenario approach used here, it is assumed that the scenario probability distribution is not known and all scenarios are assumed to be of equal probability. If an unequal scenario probability distribution is known, a stochastic MSMIOCP formulation similar to that used in this paper could be developed while using a weighted average of the constraints and the objective function, wherein the weight corresponding to a scenario is proportional to the probability of occurrence of that scenario.

In addition, using a multiple scenario approach and formulating a stochastic MSMIOCP is just one way of considering uncertainty. Uncertainty can be incorporated into an initial MSMIOCP formulation by using the other preventive methods, such as robust optimisation and parametric programming, and the resulting formulation can then be solved as a standard nonlinear optimisation problem using a procedure of the principle of Implementation II. It would be interesting to compare the results obtained using such formulations with those of the stochastic MSMIOCP formulation in this paper.

Discussion can also be drawn regarding the future applications of the approach developed in this article. While the case studies examined in this article assume that the catalyst deactivation rate constant is independent of temperature, such an assumption may not apply in applications of biochemical engineering, for example. It is sought to apply the proposed approach to optimise scheduling and production in a process while considering uncertainty in a deactivation rate parameter that is dependent on temperature.

Further, while the article here considers a process containing only a single reactor, it is common for processes to have multiple reactors operating in parallel and a recent work by Adloor and Vassiliadis (2020) considered the optimisation of maintenance scheduling and production in such a set up, but assumed all kinetic parameters involved to be known and fixed in value. It is sought to apply the proposed approach in order to understand the effects that uncertainties in kinetic parameters could have on the optimal operation of such a set up.

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Appendix A. Implementation II details

This section presents the details of Implementation II, a procedure to solve the stochastic MSMIOCP as a standard nonlinear optimisation problem, without using mixed-integer methods. This procedure was derived in a previous work by Adloor et al. (2020) to solve the deterministic version of the problem under consideration in this paper and the details presented in this section are very similar to the procedure details in that work.

In this procedure, the integer restrictions on the binary controls, $u^{(p)}$ for stage p, in equation (5f), are relaxed and these controls are instead considered as continuous variables that vary between 0 and 1. That is:

$$\begin{aligned} u^{(p)} &\in [0, 1] \\ p &= 1, 2, \ldots, NP \end{aligned} \tag{A.1}$$

Thus now, the formulation is free from binary variables and only a standard multistage optimal control problem (MSOCP) has to be solved using the feasible path approach, which can be done using any nonlinear optimisation algorithm. A penalty term homotopy technique, similar to that suggested by Sager (2005, 2009) is used to enforce the 0 or 1 values for the controls, $u^{(p)}$, for stage p. As per this technique, a monotonically increasing penalty term is added to the objective function in equation (5a) and a series of MSOCPs of the following generic form are solved:

$$F_k : \min \left[W_s + M_k \sum_{p=1}^{NP} u^{(p)} \left[1 - u^{(p)} \right] \right] \tag{A.2}$$

subject to equations (5b) – (5e), (A.1) and (5g), for

$$k = 1, 2, 3 \ldots$$

$$M_1 = 0$$

Every iteration, k, is referred to as 'major iteration'. The first major iteration ($k = 1$) of the series is designated a weight of $M_1 = 0$ and is similar to solving the problem given by equation (5), the only difference being there are no integer restrictions on controls u. If solving problem F_1 does not produce binary values for controls u, the second major iteration occurs in which a weight $M_2 > 0$ is chosen and problem F_2 is solved using the solution of F_1 as starting values. This procedure is repeated in an iterative manner, by choosing a weight $M_{k+1} > M_k$ and solving problem F_{k+1} with the solution of F_k as initial guesses, until iteration K ($K \geq 1$) such that all controls in u, in the solution of problem F_K, are forced by weight M_K to take values of either 0 or 1.

The progression for the increase of weights, M_k, is chosen arbitrarily, by trial and error, and is dependent on the parameters of the problem. It should be remembered that if the weight is increased too slowly, the computational time becomes large, while if it is increased too fast, the optimiser can fail to recognise a solution and continue iterations indefinitely.

Appendix B. Deterministic case study details

This section presents the elements of a case study of an industrial process examined in a previous work by Adloor et al. (2020). This case study was developed on the basis of an MSMIOCP formulation, of structure similar to equation (4), and is deterministic in the sense that its elements involve no parametric uncertainty. This formulation is used for the development of the MSMIOCP formulation, of the structure of equation (4), and the stochastic MSMIOCP formulation, of the structure of equation (5), of the case studies in Section 4 wherein the kinetic parameters are considered uncertain.

In the industrial problem, the following assumptions apply:

1. The industrial process operates over a fixed time horizon, in the order of years. Each year is constituted by 12 months and there are a total of NM months, wherein each month is constituted by 4 weeks.

2. The industrial process functions according to a certain process model and is subject to operating constraints.

3. The reactor containing the deactivating catalyst is a Continuous Stirred Tank Reactor (CSTR) that is of known and fixed volume.

4. The catalyst performance decays with time and has to be replaced before its activity falls below a certain minimum value.

5. The catalyst deactivation kinetics is first order with respect to the catalyst activity and is independent of the concentration of the reacting species. That is, the deactivation rate equation is of general form:

$$\frac{\mathrm{d}\,(cat\_act)}{\mathrm{d}t} = -Kd \times cat\_act \tag{B.1}$$

   where Kd is the deactivation rate constant and cat_act is the activity of the catalyst.

6. The catalyst deactivation rate constant is taken to be independent of the temperature of operation.

7. There is a maximum number of catalyst loads that can be used over the given time horizon.

8. All available catalysts exhibit identical functioning and performance.

9. The time required to shut down the process, replace the catalyst and restart the process is taken to be one month, during which time no production occurs.

10. The main reaction is assumed to be of the form:

$$R \rightarrow Q \tag{B.2}$$

   where R is the reactant and Q is the desired product. The reaction rate is considered separable from the catalyst activity and is first order with respect to the concentration of the reactant, R. That is, the reaction rate equation is of general form:

$$K_R \times cat\_act \times cR \tag{B.3}$$

where K_R is the reaction rate constant, cat_act is the catalyst activity and cR is the concentration of reactant exiting the reactor.

11. The reaction rate constant is taken to exhibit an Arrhenius form of temperature dependence.

12. The feed inlet concentration is taken to be known and constant.

13. The flow rate of raw material to the reactor has to be specified on a weekly basis.

14. The flow rate of raw material to the reactor has an upper limit during catalyst operation and is stopped when the catalyst is being replaced.

15. The temperature of the reactor has to be specified on a weekly basis.

16. The temperature of the reactor can be operated only within fixed bounds during catalyst operation and is set to its lower bound during catalyst replacement.

17. The product is produced and stored continuously as inventory.

18. The product produced is sold on a weekly basis.

19. The seasonal demand figures for the product are given.

20. The sales for each week is less than or equal to the customer demand for the product in that week.

21. There is a penalty corresponding to the unmet demand in each period.

22. The costs involved in the process are known and are subject to a known value of annual inflation. These include the sales price of the product, the cost of inventory, the cost of flow and raw material, the cost of catalyst changeover and the penalty for unmet demand.

Given the above assumptions, the optimisation model must determine the following values, which constitute the controls of the MSMIOCP:

(i) The catalyst changeover decision variable, $y(i)$, for each month, i, which determines whether a catalyst is in operation ($y(i) = 1$) or being replaced ($y(i) = 0$) during that month.

(ii) The feed flow rate to the reactor, $ffr(i, j)$, during each week, j, of each month, i.

(iii) The temperature of operation of the reactor, $T(i, j)$, during each week, j, of each month, i.

(iv) The amount of product sold, $sales(i, j)$, at the end of each week, j, of each month, i.

In the above list, $j \in \{1, 2, 3, 4\}$ and $i \in \{1, 2, ..., NM\}$. The catalyst changeover decisions correspond to the binary controls u in equation (4f) while the other decision variables correspond to continuous controls v in equation (4g).

The state variables that characterise the MSMIOCP formulation of this industrial process include

(i) the catalyst activity, cat_act

(ii) the concentration of the reactant at the exit of the reactor, cR

(iii) the inventory level, inl

(iv) the cumulative inventory costs, cum_inc

These state variables are determined by the decision variables' values at any time using a set of Ordinary Differential Equations (ODEs) which constitute the process model. In the following, ODEs of the form of equation

(4b), which apply for week $j \in \{1, 2, 3, 4\}$ of month $i \in \{1, 2, ..., NM\}$ of the process are formulated:

1. The catalyst activity decays according to a deactivation rate law given by equation (B.1) during times of catalyst operation ($y(i) = 1$) but experiences no change during times of catalyst replacement ($y(i) = 0$), when there is no production occurring. Thus, the differential equation for the catalyst activity, accounting for both scenarios, takes the form:

$$\frac{\mathrm{d}\,(cat\_act)}{\mathrm{d}t} = y(i) \times [-Kd \times cat\_act] \tag{B.4}$$

2. The reactor is assumed to be completely stirred and so the reactant exit concentration (cR) is obtained from the generic mass balance equation of a CSTR during months of catalyst operation ($y(i) = 1$), with the rate of reaction given by equation (B.3). However, during months of catalyst replacement ($y(i) = 0$), no reaction occurs and the reactor is assumed to be filled with fresh, unreacted reactant at the entry concentration ($CR0$), to be used by the new catalyst after replacement. The differential equation that accounts for both scenarios is given by:

$$\begin{aligned}\frac{\mathrm{d}\,(V \times cR)}{\mathrm{d}t} = & ffr(i,j) \times (CR0 - cR) \\ & - y(i) \times [V \times K_R \times cat\_act \times cR]\end{aligned} \tag{B.5}$$

where V is the volume of the reactor and K_R is the rate constant. Here K_R is assumed to exhibit an Arrhenius form of temperature dependence, of the form:

$$K_R = Ar \times exp\left(-\frac{Ea}{R_g \times T\,(i,j)}\right) \tag{B.6}$$

where Ar is the pre-exponential factor, Ea is the activation energy for the reaction and R_g is the universal gas constant. Equations (B.5) and

(B.6) are combined to form a single equation:

$$\frac{\mathrm{d}\,(V \times cR)}{\mathrm{d}t} = ffr(i,j) \times (CR0 - cR) - y(i) \times \left[V \times Ar \times exp\left(-\frac{Ea}{R_g \times T\,(i,j)}\right) \times cat\_act \times cR \right] \tag{B.7}$$

3. It is assumed that whatever product is produced is stored as inventory before being sold at the end of the week. During catalyst operation ($y(i) = 1$), the increase in inventory level at any time depends on the rate of production (volume times reaction rate) of the product chemical, but during catalyst replacement ($y(i) = 0$), there is no increase in inventory level. Hence, the differential equation that provides a description of the inventory level (inl) for both scenarios is given by:

$$\frac{\mathrm{d}\,(inl)}{\mathrm{d}t} = y(i) \times \left[V \times Ar \times exp\left(-\frac{Ea}{R_g \times T\,(i,j)}\right) \times cat\_act \times cR \right] \tag{B.8}$$

4. Finally, the increase in the cumulative inventory cost (cum_inc) at any time depends on the inventory level at that time and the Inventory Cost Factor (icf) (adjusted for inflation), which stipulates the cost per unit product per unit time:

$$\frac{\mathrm{d}\,(cum\_inc)}{\mathrm{d}t} = inl \times icf \tag{B.9}$$

The icf at any time is given by the following equation:

$$icf = base\_icf \times (1 + inflation)^{\lfloor i/12 \rfloor} \tag{B.10}$$

where $base\_icf$ is the inventory cost factor before inflation, $inflation$ is the annual inflation rate and $\lfloor \cdot \rfloor$ is the greatest integer function.

The set of ODEs are solved repeatedly over a weekly time span, which corresponds to one stage of the MSMIOCP. In order to solve these ODEs, for each stage, suitable initial conditions have to be provided. The initial conditions for week 1 of month 1 are assumed to be known and are of the form of equation (4c). The initial conditions for the other stages are obtained using junction conditions between two successive stages of the process, of the form of equation (4d).

The initial conditions corresponding to week 1 of month 1, represented as $init\_var(1,1)$ for variable var, are as follows:

1. The initial catalyst activity is that of a fresh catalyst ($start\_cat\_act$):

$$init\_cat\_act\,(1,1) \;=\; start\_cat\_act \tag{B.11}$$

2. At the start of the process, the reactor is filled with the reactant R at its entry concentration $CR0$. Hence, the initial exit concentration is given by:

$$init\_cR\,(1,1) \;=\; CR0 \tag{B.12}$$

3. There is no inventory at the beginning of the process, and so:

$$init\_inl\,(1,1) \;=\; 0 \tag{B.13}$$

4. There is no inventory at the start of the process and so the initial cumulative inventory cost is given by:

$$init\_cum\_inc\,(1,1) \;=\; 0 \tag{B.14}$$

The junction conditions are described next. These junction conditions differ depending on whether the catalyst is in operation $(y\,(i) = 1)$ or is being replaced $(y(i) = 0)$ during that month. In the following text, the expressions $init\_var(i,\, j)$ and $end\_var(i,\, j)$ indicate the initial and end values, respectively for the variable var, for week j of month i:

1. During months of catalyst operation $(y(i) = 1)$, the initial catalyst activity for the week corresponds to the catalyst activity at the end of the previous week. However, during months of catalyst replacement $(y(i) = 0)$, the catalyst activity has to be reset to the activity corresponding to that of a fresh catalyst, which remains the same throughout the duration of month i. The junction conditions that describe both scenarios is given by:

$$\begin{gathered} init\_cat\_act\,(i,\, j+1) \;=\; end\_cat\_act(i,\, j) \\ \forall j = 1, 2, 3 \qquad \forall i = 1, 2, \ldots, NM \end{gathered} \tag{B.15a}$$

$$\begin{aligned} init\_cat\_act\,(i,\, 1) \;&= [y(i) \times end\_cat\_act(i-1,\, 4)] \\ &\quad + [(1 - y(i)) \times start\_cat\_act] \\ &\forall i = 2, 3, \ldots, NM \end{aligned} \tag{B.15b}$$

2. During months of catalyst operation $(y(i) = 1)$, the exit concentration for the beginning of a week corresponds to the exit concentration at the end of the previous week. And during months of catalyst replacement $(y(i) = 0)$, the reactor is filled with reactant at entry concentration $CR0$, ready to be used by the fresh catalyst at the beginning of the next month. So, the junction conditions take the form:

$$\begin{gathered} init\_cR\,(i,\, j+1) \;=\; end\_cR(i,\, j) \\ \forall j = 1, 2, 3 \qquad \forall i = 1, 2, \ldots, NM \end{gathered} \tag{B.16a}$$

$$init\_cR(i,\,1) = [y(i) \times end\_cR(i-1,\,4)] + [(1-y(i)) \times CR0]$$
$$\forall i = 2, 3, \ldots, NM \tag{B.16b}$$

3. At the end of a week, an amount, $sales(i,\,j)$ of the stored product is sold. Thus, the initial inventory level for the week corresponds to the inventory present after the sales at the end of the previous week. The following junction conditions apply during months of catalyst operation as well as catalyst replacement, as the sales do not cease at any time:

$$\begin{aligned} init\_inl\,(i,\,j+1) \;&=\; end\_inl(i,\,j) - sales(i,\,j) \\ \forall j = 1, 2, 3 \qquad &\forall i = 1, 2, \ldots, NM \end{aligned} \tag{B.17a}$$

$$\begin{aligned} init\_inl\,(i,\,1) \;&=\; end\_inl(i-1,\,4) - sales\,(i-1,\,4) \\ &\forall i = 2, 3, \ldots, NM \end{aligned} \tag{B.17b}$$

4. The inventory cost accumulated until the beginning of a week is equal to the value of the inventory cost accumulated until the end of the previous week and the following junction conditions apply regardless of whether the catalyst is being used or replaced:

$$\begin{aligned} init\_cum\_inc\,(i,\,j+1) \;&=\; end\_cum\_inc(i,\,j) \\ \forall j = 1, 2, 3 \qquad &\forall i = 1, 2, \ldots, NM \end{aligned} \tag{B.18a}$$

$$\begin{aligned} init\_cum\_inc\,(i,\,1) \;&=\; end\_cum\_inc(i-1,\,4) \\ &\forall i = 2, 3, \ldots, NM \end{aligned} \tag{B.18b}$$

The initial conditions (B.11) – (B.14) and junction conditions (B.15) – (B.18) enable a solution for the ODEs for all stages, and thereby obtain the values of the state variables for the entire time horizon. These are then used to compute the values of some of the constraints and the objective function of the problem, whose formulations are described next.

The constraints, of the form equation (4e), that apply to this industrial problem for week $j \in \{1, 2, 3, 4\}$ of month $i \in \{1, 2, ..., NM\}$ are as follows:

1. In the context of solving the MSMIOCP as a series of standard MSOCPs using the feasible path approach, the catalyst changeover decision variables $y(i)$, for a month i, are considered continuous variables that vary between 0 and 1, and so the following bounds are imposed:

$$0 \;\leq\; y(i) \;\leq\; 1 \tag{B.19}$$

2. The flow rate of raw material to the reactor has an upper limit (FUp) at which it can operate. Hence, the following bounds are set on the feed flow rate for each week:

$$0 \;\leq\; ffr(i,j) \;\leq\; FUp \tag{B.20}$$

3. The sales in each week are assumed to be less than or equal to the demand for the product in that week ($demand(i, j)$). Hence, the following bounds on the sales at the end of each week are imposed:

$$0 \;\leq\; sales(i,j) \;\leq\; demand(i,j) \tag{B.21}$$

4. The temperature of the reactor operates between known, fixed lower and upper bounds, TLo and TUp, respectively. Hence, the following bounds are set on the weekly temperature of operation of the reactor:

$$TLo \;\leq\; T(i,j) \;\leq\; TUp \tag{B.22}$$

5. During times of catalyst replacement, the process is shut down and so

the flow of raw material to the reactor stops. The following constraint ensures that the weekly feed flow rate remains below the upper bound during times of catalyst operation ($y(i) = 1$) and drops to zero when there is catalyst replacement ($y(i) = 0$).

$$ffr(i,j) - [FUp \times y(i)] \;\; \leq \;\; 0 \tag{B.23}$$

6. When the process is shut down for catalyst replacement, the temperature of the reactor is required to drop to its lower bound. This condition is imposed using the following constraint which ensures that the temperature for the week remains between its bounds during times of catalyst operation ($y(i) = 1$) and drops to the lower bound when there is catalyst replacement ($y(i) = 0$):

$$TLo \;\; \leq \;\; T(i,j) \;\; \leq \;\; [(TUp - TLo) \times y(i)] + TLo \tag{B.24}$$

7. There is only a certain number of catalysts available to be used by the process. The limit on the maximum number of catalyst changeovers (n) allowed is imposed using the following constraint:

$$\sum_{i=1}^{NM} y(i) \geq NM - n \tag{B.25}$$

8. The catalyst undergoes deactivation over time and has to be replaced before it the activity falls below a certain minimum value (min_cat_act). As the the decision on whether to replace a catalyst or not is made on a monthly basis, it is sufficient to ensure that the catalyst activity does fall below this limit at the end of each month i:

$$end\_cat\_act\,(i,\,4) \;\; \geq \;\; min\_cat\_act \tag{B.26}$$

9. In order to ensure that more product than available is not sold, the inventory level at the end of each week should be greater than the sales for the week. This is imposed using the following constraint:

$$end\_inl(i,\, j) - sales(i,j) \;\; \geq \;\; 0 \qquad \text{(B.27)}$$

The objective function that represents the net costs of the industrial process, is of the form of equation (4a) and comprises the following elements:

1. The Gross Revenue from Sales (GRS)
   This term represents the revenue for the process from the net sales of the product chemical over the whole time horizon:

   $$GRS \;\; = \;\; \sum_{i=1}^{NM} \sum_{j=1}^{4} psp(i,j) \times sales(i,j) \qquad \text{(B.28)}$$

   where $psp(i,j)$ is the sales price per unit product for week j of month i, adjusted for inflation at that time:

   $$psp(i,j) \;\; = \;\; base\_psp \times (1 + inflation)^{\lfloor i/12 \rfloor} \qquad \text{(B.29)}$$

   where $base\_psp$ is the unit product sales price before inflation.

2. The Total Inventory Cost (TIC)
   This term represents the net storage costs for the product over the whole time horizon and is obtained from the solution of the ODEs for the state variable cum_inc at the end of the final week of the process:

   $$TIC \;\; = \;\; end\_cum\_inc(NM,\, 4) \qquad \text{(B.30)}$$

3. The Total Cost of Catalyst Changeovers ($TCCC$)
   The total expenditure for the catalyst changeover operations is:

$$TCCC = \sum_{i=1}^{NM} crc(i) \times (1 - y(i)) \tag{B.31}$$

where $crc(i)$ is the cost of the catalyst replacement operation for month i, adjusted for inflation at that time:

$$crc(i) = base\_crc \times (1 + inflation)^{\lfloor i/12 \rfloor} \tag{B.32}$$

where $base\_crc$ is the cost of a catalyst changeover operation before inflation. It is highlighted that the terms within the summation remain non-zero only during the times of catalyst replacement ($y(i) = 0$) and only these terms contribute to the total costs.

4. <u>The Net Penalty for Unmet Demand ($NPUD$)</u>

   The unmet demand in each week ($unmet\_demand(i,j)$) is the quantity of product by which the sales falls short of the demand in that week:

$$\begin{aligned} unmet\_demand(i,j) &= demand(i,j) - sales(i,j) \\ \forall j = 1,2,3,4 \quad &\quad \forall i = 1,2,\ldots,NM \end{aligned} \tag{B.33}$$

   There is a penalty associated with this unmet demand and the net penalty costs over the entire time horizon is given by:

$$NPUD = \sum_{i=1}^{NM} \sum_{j=1}^{4} pen(i,j) \times unmet\_demand(i,j) \tag{B.34}$$

   where $pen(i,j)$ is the penalty per unit product for week j of month i, adjusted for inflation at that time:

$$pen(i,j) = base\_pen \times (1 + inflation)^{\lfloor i/12 \rfloor} \tag{B.35}$$

   where $base\_pen$ is the penalty per unit product before inflation.

5. <u>The Total Flow Cost (TFC)</u>
   This term represents the net expenditure on the feed of raw material to the reactor and is given by:

$$TFC = \sum_{i=1}^{NM} \sum_{j=1}^{4} cof(i,j) \times ffr\,(i,j) \tag{B.36}$$

   where $cof(i,j)$ is the cost of raw material per unit volume per week for week j of month i, adjusted for inflation at that time:

$$cof(i,j) \;=\; base\_cof \times (1 + inflation)^{\lfloor i/12 \rfloor} \tag{B.37}$$

   where $base\_cof$ is the cost of raw material per unit volume per week before inflation.

If the Net Cost is represented by NC, the objective function for this optimisation problem takes the form:

$$\min NC \;=\; -GRS + TIC + TCCC + NPUD + TFC \tag{B.38}$$

This concludes the formulation of the industrial problem as an MSMIOCP, with the appropriate decision variables, state variables, differential equations, initial conditions, junction conditions, constraints and objective function. The initial MSMIOCP formulation of the case studies in Section 4, of the structure of equation (4), is equivalent to this formulation, with the exception that the kinetic parameters, Kd, Ar and Ea are uncertain. The stochastic MSMIOCP formulation, of the structure of equation (5), for optimisation of this industrial problem under uncertainty is developed in Section 4 using this MSMIOCP formulation as a basis.

Appendix C. Case Studies: Implementation details

The set of parameters that apply to all case studies are given in Table C.6. These are largely similar to the parameters used in the work by Adloor et al. (2020) that solved the deterministic version of this problem.

Table C.6: List of parameters

Parameter Symbol	Value
$\overline{Ar}$	885 (1/day)
$base\_cof$	\$ 210 /week
$base\_crc$	\$ 10^7
$base\_icf$	\$ 0.01 /(kmol day)
$base\_pen$	\$ 1250 /kmol
$base\_psp$	\$ 1000 /kmol
$CR0$	1 kmol/m^3
$demand$	1st quarter of year: 8000 kmol/week
	2nd quarter of year: 7200 kmol/week
	3rd quarter of year: 3300 kmol/week
	4th quarter of year: 4500 kmol/week
$\overline{Ea}$	30,000 J/gmol
FUp	9600 m^3/day
$inflation$	5%
$\overline{Kd}$	0.0024 (1/day)
min_cat_act	0.2983
n	5

Table C.6: List of parameters

Parameter Symbol	**Value**
NM	36 months (= 3 years)
R_g	8.314 J/(gmol.K)
$start\_cat\_act$	1
TLo	400 K
TUp	1000 K
V	50 m^3

For the given time horizon of 3 years, Table C.7 provides details of the number of decisions variables and constraints, which as mentioned previously, remain the same size as in the deterministic (single scenario) case, for all sub-problems of all case studies considered in this article. It is only the size of the ODE system that varies between the deterministic study and the case studies, and details regarding this, for the time horizon of 3 years, are given in Table C.8.

For each sub-problem in each case study, the implementation was performed in Python™ 3.7.1 under PyCharm 2019.3.3 (Community Edition). The multiple scenario values for each uncertain parameter in each sub-problem were generated by constructing sobol sequences (Sobol, 1976), of the length of the number of scenarios, within the specified range for that uncertain parameter. Using quasi-random low-discrepancy sobol sequences provided the advantage of ensuring that the range of uncertainty is covered evenly. The sobol sequences were generated using the *i4_sobol_generate* method in the *sobol_seq* module (version 0.1.2) in Python.

Table C.7: Size specifications for the decision variables and constraints, applicable for the deterministic problem as well as all sub-problems of all case studies

Property		**Size**
Decision variables	Catalyst changeover actions	36
	Feed flow rate	144
	Sales	144
	Temperature	144
	Total	*468*
Constraints	Constraints (B.19)	72
	Constraints (B.20)	288
	Constraints (B.21)	288
	Constraints (B.22)	288
	Constraints (B.23)	144
	Constraints (B.24)	288
	Constraint (B.25)	1
	Constraints (18)	36
	Constraints (19)	144
	Total	*1549*

The codes for all sub-problems were written using CasADi, an open source software that enables a symbolic framework for numerical optimisation (Andersson, 2013). The elements of the problem for all case studies, as given in Section 4, were defined as symbolic expressions using CasADi v3.5.1. The Automatic Differentiation (AD) feature of CasADi enabled constructions of symbolic expressions of the derivatives of all predefined functions, thereby maintaining differentiability to an arbitrary order. This allowed for an efficient calculation of gradients, that did not suffer from round-off and truncation errors, unlike gradient calculation using finite differences.

Table C.8: Details of the size of the ODE systems present in the deterministic problem and the sub-problems of all case studies

Case Study	**Sub-problem**	**Number of ODEs**
Deterministic problem	N/A	576
Case Study A	All sub-problems	11520
Case Study B	All sub-problems	8784
Case Study C	All sub-problems	8784
Case Study D	5 scenario sub-problem	2880
	10 scenario sub-problem	5760
	15 scenario sub-problem	8640
	20 scenario sub-problem	11520
	25 scenario sub-problem	14400

The integration of the ODEs in the feasible path approach was performed using the CasADi plug-in to the open source SUNDIALS suite (Hindmarsh et al., 2005). The *IDAS* solver of SUNDIALS was used for the integration of the ODEs with the following termination criteria: an absolute tolerance of 10^{-6} and a relative tolerance of 10^{-6}. The optimisation was performed using the CasADi plug-in to IPOPT by COIN-OR (Wächter and Biegler, 2006). The optimisation by IPOPT had, respectively, the following termination and 'acceptable' termination criteria: 10^{-4} and 10^{-4} for the optimality error, 1 and 10^{6} for the dual infeasibility, 10^{-4} and 10^{-2} for the constraint violation, and 10^{-4} and 10^{-2} for the complementarity. The 'acceptable' number of iterations was set at 15.

The implementations were performed on a 2.80 GHz Intel(R) Core(TM) i5-8400 CPU, 16 GB RAM, Windows machine running on Microsoft Windows 10 Enterprise.

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