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Optimizing the Selection of Solvents for the Dissolution and Precipitation of Polyethylene

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ABSTRACT

Plastic recycling is prevalently mechanical, which is inefficient at removing contaminants and produces low-grade materials. Solvent-based polymer dissolution and precipitation is emerging as a low-energy alternative to mechanical recycling when tackling highly contaminated plastic waste streams. We present a computer-aided molecular and process design (CAMPD) formulation for the selection of optimal solvents and process temperatures for polymer recycling via a dissolution and precipitation process. A mixed-integer nonlinear programming (MINLP) model is proposed to minimize the energy requirement for the dissolution of commercial low-density polyethylene, a ubiquitous polymer in industrial and municipal plastic waste, while minimizing the solvent viscosity and toxicity through multiobjective optimization. We integrate the SAFT-γ Mie group-contribution equation of state in the optimization framework to predict key thermodynamic properties and to ensure that the desired phase behaviour is achieved. A ranked list of solvents and the corresponding process temperatures is obtained using integer cuts. Two polyethylene molecular weights are considered. In each case, we construct a Pareto front to quantify the trade-offs between the energy requirements of the process and the selected solvent properties. Furthermore, we investigate the simultaneous design of the dissolution and cooling precipitation to analyse the effect of varying the precipitation temperature on the energy of dissolution. The current study provides valuable insights into selecting optimal solvents for polyethylene dissolution, advancing the design of more efficient plastic recycling processes.

Keywords: Plastic recycling, CAMPD, SAFT-γ Mie.

INTRODUCTION

The recycling of plastics via solvent-based processes is an emerging alternative to the more established mechanical recycling technologies, particularly when addressing highly contaminated and multilayer plastic waste, and targeting high-quality recycled polymers [1]. Amongst solvent-based recycling technologies, physical recycling processes, that do not involve any chemical modifications of the molecular species, lead to significantly less carbon dioxide (CO_2) emissions compared to chemical recycling, which requires the energy-intensive cleavage of polymer bonds to produce monomers, the building blocks of polymers [2]. This is particularly the case when considering polyolefins like polyethylene and polypropylene, which have highly unreactive carbon-carbon bonds. However, dissolution and precipitation methods are more energy intensive than mechanical recycling and are often not suitable to produce food-grade recycled polymers due to the use of toxic solvents [3], which also pose general concerns with respect to environmental impact. Identifying new solvents and improved process designs is therefore key to advancing solvent-based dissolution and precipitation to levels comparable with mechanical recycling and to make it competitive with virgin polymer production.

Polymer solubility experiments are expensive and time consuming, so that the availability of predictive tools

for relevant properties to make informed decisions about the process and solvent choice is critical. The selection of solvents based on Hansen solubility parameters (HSPs) has been proposed [4]. While HSPs are useful for rapid solvent screening, they do not provide the required properties for process optimization, such as the solubility or the enthalpy at different process conditions. Recently, COSMO-RS, which can account for polymer–solvent molecular detail, has been used to predict the solubility of polymers in solvents for dissolution applications [5]. However, the prediction of the solubility of the polymer with COSMO-RS is computationally expensive, requiring molecular simulation to identify representative polymer conformations. Furthermore, there has been limited validation of the approach in terms of the polymer molecular weight and of the temperature range. The SAFT-γ Mie [6,7] equation of state offers an alternative route to predict solid–liquid equilibrium and liquid–liquid demixing in polymer-solvent mixtures, as well as other thermodynamic properties. It has been shown to deliver accurate properties of complex mixtures, including polymers and solvents [6-8], and, as a group-contribution method, it is naturally suited for use in solvent (molecular) design. It has for example recently been used in computer-aided molecular and process design (CAMPD) to identify better solvents and process conditions for pharmaceutical manufacturing [9] and for CO_2 capture [10]. Crystallization processes in drug manufacturing also depend heavily on solubility (solid–liquid equilibrium), providing a foundation for the model-based design of dissolution-precipitation processes. The use of SAFT-γ Mie to support the design of physical recycling processes is investigated in our current study, building on previous work on multiobjective optimization (MOO) to understand the tradeoffs between different objective functions, such as the solvent toxicity [11], the crystal yield and the solvent consumption [9].

The CAMPD framework is applied for the first time to solvent-based dissolution and precipitation recycling of plastics. As case studies, we explore the selection of optimal solvents and process conditions that minimize the energy requirements for the recycling of two types of low-density polyethylene (LDPE) while ensuring a homogeneous liquid polymer–solvent mixture is formed. This scenario is relevant to a plastic recycling problem where LDPE is mixed with solid waste impurities, such as secondary plastics and the presence of metals or cardboard [12]. We provide a ranked list of optimal solvents and process conditions and explore the trade-offs between the energy requirements and two key solvent properties: toxicity and viscosity. Furthermore, we analyse the relationship between the objective function and the precipitation temperature.

DESIGN METHODOLOGY

Problem definition

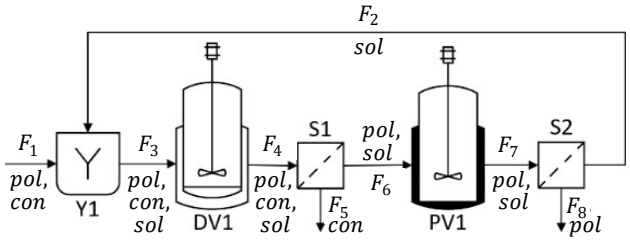

Figure 1: Schematic of an idealised polyethylene dissolution and cooling precipitation flowsheet.

In the CAMPD problem we focus on a general approach to designing a polymer dissolution and precipitation system. This involves identifying the optimal solvent molecules, weight fractions, and process temperatures to minimize the performance objective, which in this case is the energy of dissolution. The process configuration is shown in Figure 1, assuming perfect separation in each unit. A stream of plastic waste consisting of LDPE (pol) and a solid contaminant (con), with a flowrate F_1 , is mixed with a solvent (sol) recycle stream F_2 in a mixer Y1. The two-phase slurry F_3 is fed to a dissolution vessel DV1, where heat is provided through a heating jacket to dissolve the solid polymer. The outlet of DV1 is passed through a filtration unit S1, where the undissolved solid contaminants are filtered out. The filtrate F_6 then enters a precipitation vessel PV1, where the polymer–solvent mixture is cooled down to obtain solid polymer. Finally, the solvent is recovered in filter S2, and the purified

Table 1: Key model equations.

Description	Equation	
Energy consumption	$Q = Q_{pol} + \left[F_4^L\, h^L(T_4, P_4, x_4^L) - F_3^L x_{3,pol}^L h_{pol}^L(T_3, P_3) - F_3^L x_{3,sol}^L h_{sol}^L(T_3, P_3)\right]$	(1)
Heat required to obtain a liquid polymer at T_3	$Q_{pol} = F_3^s x_{3,pol}^s [c_{P,pol}^S (T_{pol}^{\text{fus}} - T_3) + \Delta h_{pol}^{\text{fus}}] + F_3^L x_{3,pol}^L [h_{pol}^L(T_3, P_3) - h_{pol}^L(T_{pol}^{\text{fus}}, P_3)]$	(2)
Solid–liquid equilibrium model	$\ln \boldsymbol{x}_{i,pol}^L + \ln \gamma_{i,pol}(T_i, P_i, \boldsymbol{x}_i^L) = -\frac{\Delta h_{pol}^{\text{fus}}}{R}\left[\frac{1}{T_i} - \frac{1}{T_{pol}^{\text{fus}}}\right],\ i = 4{,}7,\ 0 \le w_{7,pol}^L \le 10^{-6}$	(3)
Polymer and solvent form a single stable liquid phase	$\tilde{S}_l\ (T_4, P_4\ , x_4^L) = 1$	(4)

polymer leaves S2 in stream F_8.

Model formulation

All separations are assumed to be perfect. The polymer is a solid in streams $1, 3, 7,$ and 8, and in the liquid phase in streams 4 and 6. Stream 2 is pure solvent, stream 5 pure solid contaminant and stream 8 pure polymer. The material balances for the system are easily derived and not shown.

Other key model equations are shown in Table 1. Q is the energy consumption in dissolution vessel DV1, neglecting any energy required for agitation as well as the enthalpy change due to the solid contaminant. It is derived from an energy balance around DV1, given as Equations (1) and (2) in Table 1, where F_i^L denotes the liquid flowrate in stream i, F_i^S the corresponding solid flowrate, and $h_i^L(T_i, P_i, \boldsymbol{x}_i^L)$ the liquid-phase enthalpy of stream i at temperature T_i, pressure P_i (here assumed to be atmospheric throughout) and mole fraction vector $\boldsymbol{x}_i^L$. $h_{i,pol}^L$ and $h_{i,sol}^L$ denote the pure component liquid-phase enthalpies for the polymer and the solvent, respectively. $\boldsymbol{x}_{i,k}^L$ denotes the mole fraction of component k (pol or sol) in the liquid phase in stream i, while $\boldsymbol{x}_{i,pol}^S$ denotes the corresponding solid-phase mole fraction. Q_{pol} is the enthalpy change of the polymer on going from solid to liquid. $c_{P,pol}^S$ is the solid-phase molar heat capacity of the polymer, T_{pol}^{fus} is the melting temperature of the polymer, and $\Delta h_{pol}^{\text{fus}}$, its enthalpy of fusion at T_{pol}^{fus}.

Solid–liquid equilibrium must hold in DV1 and PV1. This is enforced by Equation (3). $\gamma_{i,pol}(T_i, P_i, \boldsymbol{x}_i^L)$ is the activity coefficient of the polymer at the specified conditions, and R is the ideal gas constant. In addition, the mass fraction of polymer in the liquid phase in PV1 (i.e., in F_7^L) is set to be very close to zero to ensure full precipitation.

Finally, in order to ensure that the polymer and solvent form a single stable liquid phase in DV1, a logical stability function $\tilde{S}_l$ $(T_4, P_4, \boldsymbol{x}_4^L)$ is constrained to 1. A value of 1 indicates that a temperature-pressure flash calculation at the specified conditions does not detect a second liquid phase or a vapour, while 0 indicates the presence of another fluid phase.

SAFT-γ Mie is used to calculate the activity coefficients and the liquid-phase enthalpies with group interaction parameters taken from [8] or combining rules [8] where no group parameters have been developed.

CAMPD formulation

The model equations are integrated within a Mixed Integer Nonlinear Programming (MINLP) that takes as input a list $\mathcal{L}$ of candidate solvents. Each solvent l is characterized by a set of functional group numbers, $n_{g,l}$, $g \in G$, where G is the set of SAFT-γ Mie groups, as well as its toxicity τ_l, taken as LC_{50} from [16], and an experimental viscosity η at $298\ \text{K}$, taken from the DETHERM database [17]. A binary variable y_l is introduced to denote whether solvent candidate l is selected and is defined such that only one solvent can be chosen:

$$\sum_{l \in \mathcal{L}} y_l = 1. \tag{5}$$

Assignment constraints are used to set the values of the SAFT-γ Mie group numbers, the toxicity, and the viscosity to be those of the selected solvent. The number of groups of type g in the solvent is given by

$$n_g = \sum\nolimits_{l \in \mathcal{L}} y_l n_{g,l}, \tag{6}$$

and the toxicity and viscosity are given by

$$\tau = \sum\nolimits_{l \in \mathcal{L}} y_l \tau_l; \quad \eta = \sum\nolimits_{l \in \mathcal{L}} y_l \eta_l \tag{7,8}$$

A constraint is also imposed on the maximum mass fraction of polymer in DV1, to prevent the formation of gel.

The problem is formulated using up to two objectives that must be minimized, one of which is always Q and the other τ or η.

CASE STUDIES

Case study description

LDPE is one of the most widely present polyolefins in plastic products and is highly valued for its durability and versatile nature. However, its durable qualities make its recycling challenging and energy intensive. Two molecular weights of polymer are considered, $270\ \text{kg mol}^{-1}$ and $4\ \text{kg mol}^{-1}$, and the designs are developed on a basis of $1\ \text{kg}$ of polymer. The primary objective of the design problems considered is to identify optimal solvents and corresponding process conditions to minimize the energy consumption, Q, in a process to remove a solid contaminant from LDPE via dissolution-precipitation. A secondary objective is also considered in some cases, chosen as either the minimization of the toxicity τ or of the viscosity η.

The specific heat capacity $c_{P,pol}^S$ is assumed to be independent of molecular weight and set equal to the experimental value measured at $1\ \text{atm}$ and $298\ \text{K}$, $46.5\ \text{J mol}^{-1}\ \text{K}^{-1}$ [15]. The experimental values for T_{pol}^{fus} values are either obtained through differential scanning calorimetry (DSC) in our current work or from [13], and the experimental values for $\Delta h_{pol}^{\text{fus}}$ are obtained from [14] (see Table 2).

Polythermal solubility measurements are conducted for selected polymer-solvent mixtures, corroborating the reliability of the SAFT-γ Mie model.

Table 3: Ranking of optimal solvents generated with integer cuts for both polymers considered. Energy consumption (Q), polymer mass fraction (w), dissolution temperature (T_4), mixture stability ($\tilde{S}_l$), solvent toxicity (τ) [16], and viscosity (η) [17] at the solution of the CAMPD problem with T_7 =298.15 K.

LDPE	Rank	Solvent selected?	Q/kJ	w_{pol}	T_4 /K	$\tau(-\log[\mathrm{LC}_{50}])$	η / (mPa s)
4 kg mol^{-1}	1	Decalin	366.03	0.3	341.05	3.88	2.47
	2	Mesitylene	401.38	0.3	343.42	4.19	0.66
	3	Xylene	404.74	0.3	344.17	3.81	0.61
	4	Toluene	420.01	0.3	346.41	3.42	0.55
	5	Benzene	455.88	0.3	351.21	3.61	0.82
270 kg mol^{-1}	1	Decalin	439.04	0.3	356.07	3.88	2.47
	2	Mesitylene	458.70	0.3	356.33	4.19	0.66
	3	Xylene	462.83	0.3	357.31	3.81	0.61
	4	Toluene	479.05	0.3	359.85	3.42	0.55
	5	Cymene	582.59	0.3	373.93	3.61	0.82

Table 2: Molecular weight and melting properties of the polymers of interest [14]. [*] denotes the property is measured in our current work.

	Short LDPE	**Long LDPE**
$\boldsymbol{M_w/(\mathrm{kg\ mol^{-1}})}$	4	270
$\boldsymbol{u}$ /(-)	142	9623
$\boldsymbol{T_i^{\mathrm{fus}}/\mathrm{K}}$	375.15 [*]	389.15 [13]
$\boldsymbol{\Delta h_i^{\mathrm{fus}}/(\mathrm{kJ\ mol^{-1}})}$	8.22u [14]	8.22u [14]

To construct the list of candidate solvents we conduct an HSP analysis to identify solvents that exhibit low relative energy difference (RED) values with LDPE, using a threshold of 0. The solvents used in dissolution and precipitation experimental studies reported by Li et al. [1] and Ügdüler et al. [4] are considered. This results in 17 candidate molecules. To evaluate the effects of the precipitation temperature (T_7) on the design problem, ten design scenarios are considered with different allowed temperature differences between DV1 and PV1.

Results and discussion

The formulation is implemented in gPROMS Process version 2023.1.0 and solved using the MINLPOA (outer approximation) local solver. The built-in stability function is used for Equation (4).

The ranked list of optimal solutions shown in Table 3, obtained for a base case of $T_7 = 298.15$ K, indicates that decalin, mesitylene, xylene, toluene, benzene and cymene are promising solvent candidates that require the least energy to dissolve LDPE. The first four solvents are the same for both polymer samples, while benzene and cymene rank fifth for the $4\ \mathrm{kg\ mol^{-1}}$ LDPE and 270 kg mol^{-1} LDPE, respectively. The polymer solubility (w_{pol}) reaches the 0.30 upper bound in each iteration, indicating that high solubility and, thus, low solvent use minimizes the energy requirements of the process. Trade-offs between Q and τ, and between Q and η, are explored by solving bi-objective problem using the ε-constraint

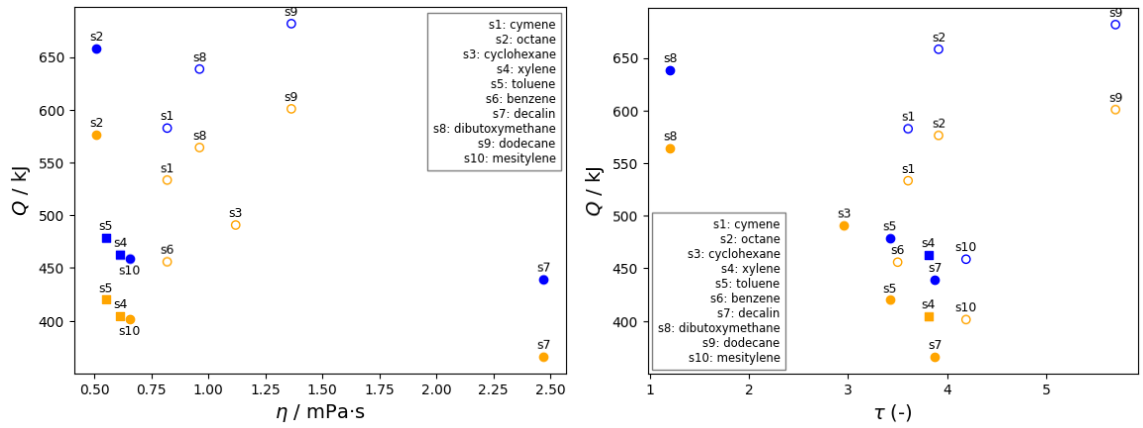

Figure 2: Pareto optimal solutions (filled circles) obtained when solving the optimization problem with two competing objectives: energy consumption Q and solvent viscosity η (left), and energy consumption Q and solvent toxicity τ (right). Empty circles depict feasible solvents. The colour indicates the type of polymer: 270 kg mol^{-1} polyethylene (blue) and 4 kg mol^{-1} polyethylene (orange). Note that the filled circles denote Pareto points found via the ε-constraint method and the filled squares Pareto points found only via integer cuts due to the ε steps.

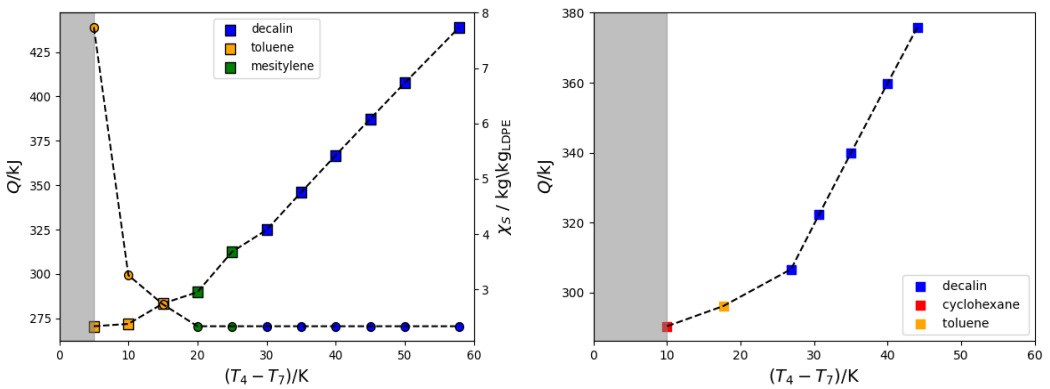

Figure 3: Minimum energy requirement Q as a function of the minimum allowed temperature difference between dissolution and precipitation $(T_4 - T_7)$ for 270 kg mol^{-1} LPDE (left plot) and 4 kg mol^{-1} LPDE (right plot). χ_S indicates the solvent inventory. The point with the largest value of $(T_4 - T_7)$ corresponds to the temperature difference when T_7 =298.15 K. Gray shading indicates infeasible regions. The dashed curves are included to aid visualisation.

method for 10 equally spaced ε values. Pareto optimal solvents are depicted in Figure 2, together with feasible solvents. These were obtained by adding integer cut inequality constraints to the optimization problem. According to the Multi Objective Optimization (MOO) solutions, mesitylene may be a more suitable solvent to dissolve polyethylene than decalin due to its significantly lower η with only a slightly higher Q. A solvent with a lower viscosity is desirable as it may offer faster dissolution and lower processing costs due to a lower energy input for pumping and mixing. On the other hand, no solvent offers a significantly lower toxicity than decalin without a large increase in energy requirements. However, toxicity may be considered less critical than viscosity if the polymer is fully recovered and the solvent is efficiently recycled, minimizing solvent loss to the environment. Employing cymene, a bio-derived solvent that ranks fifth (cf. Table 3) for $270\ \mathrm{kg\ mol^{-1}}$ LDPE, offers a potentially sustainable alternative to conventional organic solvents by reducing the reliance on fossil feedstocks for solvent production—aligning with the core objective of polymer recycling to promote environmental sustainability. On the other hand, a high recycling efficiency can reduce the greenhouse gas emissions associated with the need for fresh solvent input, potentially justifying the use of conventional organic solvents, particularly if they contribute to lower overall process energy demands. A broader lifecycle analysis is required to quantify these trade-offs. Dibutoxymethane, the least toxic solvent considered is associated with a high energy consumption, likely due to its polarity. An expanded solvent design space may help us to identify additional feasible solvents and explore the empty regions of the multiobjective spaces shown in Figure 2. This could be achieved by allowing the design of solvent mixtures [18].

The impact of the precipitation temperature, T_7, on the energy consumption is investigated by varying the temperature limit constraint. As shown in Figure 3, by reducing the extent of cooling in PV1, the optimal solvent, toluene for $270\ \mathrm{kg\ mol^{-1}}$ LDPE and cyclohexane for $4\ \mathrm{kg\ mol^{-1}}$ LDPE, can be supplied to DV1 at a higher temperature and thus the energy consumption decreases. This trend is a result of the steep decrease in solubility of LDPE as a function of temperature in the vicinity of the pure solvent limit. Based on the analysis in Figure 3, the optimal operating temperatures for PV1 are $347.19\ \mathrm{K}$ for $270\ \mathrm{kg\ mol^{-1}}$ LDPE and $342.54\ \mathrm{K}$ for $4\ \mathrm{kg\ mol^{-1}}$ LDPE when a margin of at least 5 K between T_4 and T_7 is enforced. These guarantee 100% LDPE precipitation and energy requirements of $283.32\ \mathrm{kJ}$ and $290.37\ \mathrm{kJ}$ for 270 and $4\ \mathrm{kg\ mol^{-1}}$ LDPE, respectively. The operating point for $270\ \mathrm{kg\ mol^{-1}}$ LDPE offers a good compromise between Q and a solvent inventory (χ_S) equal to 3.26. While for all $4\ \mathrm{kg\ mol^{-1}}$ LDPE points a χ_S of 2.33 is achieved.

CONCLUSIONS

We have developed a general formulation for the optimal process and solvent design for solvent-based dissolution and precipitation recycling of plastics based on a CAMPD framework with a simple initial process model and rigorous thermodynamics. In this framework, the optimal solvent candidate, the polymer solubility, and the dissolution (and precipitation) temperatures required to minimize the energy consumption can be obtained simultaneously. The general model is applied to the dissolution and precipitation of two types of LDPE, for which separate ranked lists of optimal solvents are produced. In both cases, only apolar solvents appear in the solvent rankings, with decalin identified as minimizing the energy consumption. MOO is employed to consider the trade-offs between the energy consumption and toxicity or viscosity of the solvent. Mesitylene is found to have a lower viscosity and similar Q when compared to decalin. The

simultaneous optimization of the dissolution and precipitation temperatures leads to improved results when compared to the case where the precipitation temperature is fixed and highlight the impact on the solvent inventory, which also has implications on the cost and environmental impact of the process and have not yet been quantified.

The current study provides a foundation for optimizing the dissolution-precipitation process, to make this recycling technology both economically viable and environmentally friendly. In future work, we plan to extend the design formulation to treat multilayer plastic waste, including polyethylene mixed with polypropylene, and solvent mixtures. We also aim to include a technoeconomic and lifecycle analysis for a more advanced flowsheet of the physical recycling process.

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