Expert Systems with Applications 40 (2013) 4496–4502

Contents lists available at SciVerse ScienceDirect

Expert Systems with Applications

journal homepage: www.elsevier.com/locate/eswa

Parameter estimation of a pressure swing adsorption model for air separation using multi-objective optimisation and support vector regression model

Yang Liu [a,*], Fan Sun [b]

[a] Department of Engineering, Edinburgh University, EH9 3JL, UK
[b] Intelligent Systems Research Centre, University of Ulster, BT48 J7L, UK

ARTICLE INFO

Keywords:
Parameter estimation
Multi-objective optimisation
Support vector machine

ABSTRACT

In order to successfully estimate parameters of a numerical model, multiple criteria should be considered. Multi-objective Differential Evolution (MODE) and Multi-objective Genetic Algorithm (MOGA) have proved effective in numerous such applications, where most of the techniques relying on the condition of Pareto efficiency to compare different solutions. We describe the performance of two population based search algorithms (Nondominated Sorting Differential Evolution (NSDE) and Nondominated Sorting Genetic Algorithm (NGAII)) when applied to parameter estimation of a pressure swing adsorption (PSA) model. Full PSA mode is a complicated dynamic processing involving all transfer phenomena (mass, heat and momentum transfer) and has proven to be successful in a wide of applications. The limitation of using full PSA models is their expensive computational requirement. The parameter estimation analysis usually needs to run the numerical model and evaluate the performance thousands of times. However, in real world applications, there is simply not enough time and resources to perform such a huge number of model runs. In this study, a computational framework, known as v-support vector regression (v-SVR) PSA model, is presented for solving computationally expensive simulation problems. Formulation of an automatic parameter estimation strategy for the PSA model is outline. The simulations show that the NSDE is able to find better spread of solutions and better convergence near the true Pareto-optimal front compared to NSGAII-one elitist MOGA that pays special attention to creating a diverse Pareto-optimal front.
© 2013 Elsevier Ltd. All rights reserved.

1. Introduction

Pressure Swing Adsorption (PSA) has found a wide range of applications in air drying, separation of oxygen and nitrogen in air, hydrogen purification, solvent vapour recovery and various separations in which it is difficult to separate by other common techniques, such as distillation and extraction. After its invention, a great deal of theoretical and experimental researches have been focused on PSA modelling with the growth in computing power (Farooq, 1988; Hassan, Raghavan, & Ruthven, 1986; Hassan, Raghavan, & Ruthven, 1987; Ruthven, 1984; Sankararato & Gupta, 2007). They give a good description of the dynamic processes since they cater for mass, momentum, and heat conservation.

Parameter estimation is the process of modifying the input parameters to a numerical model until the output from the model matches an observed set of data. In automatic parameter estimation, parameters are adjusted automatically according to a specified search scheme and numerical measures of the goodness-of-fit (Liu, 2009; Madsen, 2000). Compared to manual parameter estimation, automatic parameter estimation is faster while being objective and relatively easy to implement. It has been found that success of model parameter estimation depends on the choice of the objective function used (Cooper, Nguyen, & Nicell, 1997; Janssen & Heuberger, 1995). For a more detailed description about performance measures for comparing model predictions and observations using different objective functions the reader is referred to Janssen and Heuberger (1995). Many real-world optimisation problems, especially numerical parameter estimation situations, require the process of simultaneous optimisation of possibly conflicting multiple objectives, and this is termed multi-objective optimisation. The multi-objective chemical model parameter estimation problem can be stated as the optimisation problem:

$$\text{Minimize} \quad F(\theta) = \{f_1(\theta), f_2(\theta), \ldots, f_m(\theta)\} \tag{1}$$

where $f_1(\theta), f_2(\theta), \ldots, f_m(\theta)$ are the m non-commensurable objective functions to be simultaneously minimized with respect to the parameters θ of the model (Yapo, Gupta, & Sorooshian, 1998). By definition, the multi-objective optimisation has a very different nature from that of a single-objective optimisation. Unlike single-objective optimisation where only one optimal solution is pursued, a typical multi-objective optimisation problem produces a set of solutions which are superior to the rest of the solutions with respect to all objective criteria but are inferior to other solutions in one or

* Corresponding author.
E-mail address: sharkyangliu916@hotmail.com (Y. Liu).

0957-4174/$ - see front matter © 2013 Elsevier Ltd. All rights reserved.
http://dx.doi.org/10.1016/j.eswa.2013.01.054

more objectives. These solutions are known as Pareto optimal solutions or non-dominated solutions. In the absence of additional information, it is not possible to distinguish any one of the Pareto solutions as being objectively better than any others with respect to all the objectives concerned (i.e. there is no uniquely "best" solution); therefore, any one of them is an acceptable solution (Yapo et al., 1998). Once the set of optimal solutions is identified, the designers have the freedom of choosing one solution out of many possible solutions based on their experience and prior knowledge and other criteria or constraints. Most multi-objective techniques attempt to identify a set of optimal solutions which represent the trade-off surface between conflicting criteria. Practical experience with model parameter estimation suggests that no single objective function is adequate to measure properly the simulation of all the important characteristics of the system that are reflected in the observations. Therefore, there is a need to consider multiple objectives for model parameter estimation to be effective.

Genetic Algorithms (GAs) are becoming popular choices for better global optimisation frameworks to fully realise the full benefits to conducting numerical model parameter estimation, because of their simplicity, global perspective, and inherent parallel processing (Deb, 2001; Goldberg, 1989; Holland, 1975). Genetic algorithms attempt to mimic the natural selection process to optimise a target function. The capabilities of multi-objective genetic algorithms (MOGAs) to explore and discover Pareto-optimal fronts on multi-objective optimisation problems have been well recognised (Deb, Agrawal, Pratap, & Meyarivan, 2002; Liu, 2009). It has been shown that MOGAs outperform traditional deterministic methods to this type of problem due to their capacity to explore and combine various solutions to find the Pareto front in a single run. The NSGA-II optimisation algorithm has been shown to provide an efficient approximation of the Pareto front for the design of pressure swing adsorption (Fiandaca, Fraga, & Brandani, 2009). Fiandaca et al. (2009) presented an investigation of a fast cycle PSA operation, the separation of air for N2 production. The two-objective optimisation problems (the recovery of N2 achieved and the purity of the N2 actually recovered) are formulated for the operation of a PSA. The simulation requires a diffusion model, which involves coupled non-linear partial differential and algebraic equations (PDAES). The simulation results suggest that the proposed optimisation framework is able to achieve good solutions as well diversity using NSGA-II. The simulated annealing method is based on an analogy between the way in which solids cool and anneal and the optimisation of a function with many degrees of freedom. The annealing of a solid is accomplished by heating it up and allowing it to cool down slowly so that thermal equilibrium is maintained. This ensures that the atoms are obtaining a minimum energy state. An advantage of SA is that it can handle mixed discrete and continues problems. Sankararato and Gupta (2007) developed a modified multi-objective simulated annealing (MOSM) optimisation and applied it to optimise 6 operation parameters (adsorption pressure, desorption pressure, adsorption and purge times, and input flow rate) of a two-fixed-bed, four-stage pressure swing adsorber (PSA) unit for separation of air. Four objective functions (Purity of O2, Recovery rate of O2, Purity of N2 and Recovery rate of N2) were applied using the MOSM and the optimal Pareto front was achieved using the MOSM. However, each simulation of PSA model took around 24 h to attain cyclic stable state (CSS) and the CPU time required for solving the four-objective optimisation problems on a Pentium 4 (2.99 GHz) is 720 h with this algorithm. Sankararato and Yoo (2011) described details of the rMOSA algorithm. Four computationally intensive benchmark problems and on simulation-intensive two-objective problem for an industrial fluidized-Bed Catalytic Cracking Unit (FCCU) are solved using the newly developed algorithms (rMOSA and Simple MOSA) and two well-known existing MOO algorithms (NSGA-II-JG and NSGAII). The developed rMOSA was proved to converge to Pareto sets in less number of simulations with well-crowed uniform non-dominating solutions in them, for the problems considered in their study. The particle swarm optimisation and differential evolution are two new stochastic optimisation methods minimizing an objective function that can model the problem's objectives while incorporating constraints, and have three main advantages: global search regardless of the initial parameter values, fast convergence, and few control parameters. Both techniques have shown great promise in several real-world applications (Eberhart & Shi, 2000; Kennedy & Eberhart, 1995; Storn & Price, 1995). DE and PSO seem particularly suitable for multi-objective optimisation mainly because of the high speed of convergence (Coello, Pulido, & Lechuga, 2004; Lorio & Li, 2004). The non-dominated sorting differential evolution (NSDE) and non-dominated sorting particle swarm optimisation (NSPSO) combine the advanced operations (fast ranking of non-dominated solutions, crowding distance ranking, elitist strategy of combining parent population and offspring population together, selection and mutation operations) with a single DE and a single PSO (Deb et al., 2002; Liu, 2009; Lorio & Li, 2004).

The study case was modelled using the rigorous model which comprises unsteady mass and energy balance equations for the macro-voids (gas "phase"), as well as mass balance equations for the micro-voids (inside the porous particle "phase") (Sankararato & Gupta, 2007). The rigorous model has advantages over the more popular linear driving force (LDF) model in that slightly better (non oscillatory) results are obtained with fewer finite-difference grid points. However, the limitation of using full PSA models is their expensive computational requirement. Liu, Pender, and Neélz (2009) proposed a nonlinear regression model (Support vector machine) using machine learning technique to predict the 2D fluid dynamic model results obtained from a very small number of fine grid model runs instead of running the time consuming fluid dynamic model. We adopted this idea in this paper and the work presents an integration of v-SVR by using a very small number of fine grid PSA model runs to estimate purity and recovery rate of the O_2 for air separation after the training process. In the following we refer to this technique as v-SVR-PSA model. If adequately trained, the algorithm reported can serve as an alternative to expensive PSA models for fitness estimation during parameter estimation process. This approach can substantially reduce the computational time without compromising the predictive capabilities of a fine grid PSA model. The parameters of the PSA models cannot, in general, be determined directly from physical characteristics, and hence the parameter values must be estimated by parameter estimation against observed data. In this paper, the multi-objective optimisation problems are formulated for a PSA system using the recent and efficient algorithm (NSDE). The multi-objective parameter estimation of the v-SVR-PSA model shows that the NSDE is able to find better spread of solutions and better convergence near the true Pareto-optimal front compared to NSGAII-one elitist MOGA that pays special attention to creating a diverse Pareto-optimal front.

2. Pressure swing adsorption model evaluation using support vector machine

Two fixed bed adsorbers are used, as shown schematically in Fig. 1. This is basic Skarstrom PSA cycle and each bed undergoes a cyclic operation (see in Fig. 2) involving four stages (pressurization, adsorption, blowdown and purge) (Skarstorm, 1960). The CPU time required for simulation (to attain CSS, for the 6 decision variables) on an Intel core 2 Quad CPU 2.30 GHz and 3 GB of RAM is around 12 h. Details of this unit are given in Table 1 (Sankararato & Gupta, 2007). The source code of rigorous model was developed in

دریافت فوری ← متن کامل مقاله

ISIArticles
مرجع مقالات تخصصی ایران

✓ امکان دانلود نسخه تمام متن مقالات انگلیسی
✓ امکان دانلود نسخه ترجمه شده مقالات
✓ پذیرش سفارش ترجمه تخصصی
✓ امکان جستجو در آرشیو جامعی از صدها موضوع و هزاران مقاله
✓ امکان دانلود رایگان ۲ صفحه اول هر مقاله
✓ امکان پرداخت اینترنتی با کلیه کارت های عضو شتاب
✓ دانلود فوری مقاله پس از پرداخت آنلاین
✓ پشتیبانی کامل خرید با بهره مندی از سیستم هوشمند رهگیری سفارشات