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Application of the bio-inspired Krill Herd optimization technique to phase equilibrium calculations

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ABSTRACT

The Krill Herd optimization technique, which is based on the simulated herding behaviour of the krill crustacean, is applied to calculations involving phase equilibrium and phase stability, as the application of this emerging technique is extremely limited in the literature. In this work, the Krill Herd algorithm (KH)[1] and the modified Lévy-flight Krill Herd algorithm (LKH)[2] has been applied to phase stability (PS)[3] and phase equilibrium calculations in non-reactive (PE)[4] and reactive (rPE)[5] systems, where global minimization of the total Gibbs energy is necessary. Several phase stability and phase equilibrium systems were considered for the analysis of the performance of the technique that includes both vapour and liquid phase conditions.

The Krill Herd algorithm was found to reliably determine the desired global optima in PS, PE and rPE problems with generally higher success rates and lower computing time requirements than previously applied metaheuristic techniques such as those involving swarm intelligence and genetic and evolutionary algorithms.

1. Introduction

The behaviour of a particular system of components at a fixed temperature (T), pressure (P) and overall composition (z_i) is essential for the design and simulation of most processes involving the system. Particularly from a chemical engineering stand point, the knowledge of the phase behaviour of a system of components is imperative for the design and simulation of the majority of separation processes. Such processes can include complex techniques such as reactive distillation and supercritical extraction, where the accuracies and reliabilities of phase behaviour calculations have a strong influence on the simulation results (Seider and Widagdo, 1996).

The phase behaviour of a mixture at a fixed T, P, z_i, is generally characterized by phase stability (PS) and phase equilibrium (PE) (Wakeham and Stateva, 2004). The phase stability (PS) problem requires the calculation of the number of phases a particular closed system at a given T, P and z_i will form in order to achieve the state of its lowest total Gibbs energy (G^t). A system is stable if, for instance, a mixture of two liquids forms a single liquid phase at a fixed temperature, pressure and overall composition.

A consequence of instability is of course the formation of two or more phases that equilibrate at the closed system temperature and pressure. This leads to the phase equilibrium (PE) calculation where the composition and volume of each phase must be determined to characterize the phase behaviour of the entire system.

It is also possible that a chemical reaction may occur between the constituents of the mixture under consideration. In such cases additional species are generated by the chemical reaction. The phase behaviour is thus influenced by the reaction kinetics, and conversely, the reaction equilibrium is influenced by the phase behaviour (composition and volume at phase equilibrium). These type of systems exhibit simultaneous chemical (reactive) and physical equilibrium (phase) (rPE).

The phase stability problem requires the global minimization of the tangent plane distance function (TPDF) (discussed in Section 3), which is used to indicate the stability of a system for a given T, P and z_i. The PE and rPE problems require the global minimization of the total Gibbs free energy. These optimizations have proven to be challenging (Zhang et al., 2011a,b). This is due to several

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[1] Krill Herd algorithm.
[2] Lévy-flight Krill Herd algorithm.
[3] Phase stability.
[4] Phase equilibrium.
[5] Reactive phase equilibrium.

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Nomenclature

Symbols

c	total number of components in a mixture
C_{best}	effective coefficient of best krill
C_{food}	food attraction coefficient
D_i	random diffusion variable of ith individual
F_i	foraging variable of ith individual
g	Gibbs energy change of mixing
G^E	Gibbs excess energy
ΔG_{rxs}°	standard Gibbs energy change of reaction
GSR	global success rate
G_T	total Gibbs energy
h	Krill generation
K_{eq}	reaction equilibrium constant
K^{eq}	vector of reaction equilibrium constants
K_i	value of objective function of ith individual
K_{best}	optimum value of the objective function K
$\widehat{K}_{i,j}$	relative fitness of the evaluated objective function, K of the ith and jth individuals.
$\widehat{K}_{i,ibest}$	relative fitness of the current evaluated objective function, K of the ith individual with its previous best value
K_{worst}	worst value of the objective function K
k^{max}	maximum number of allowable iterations for the calculation
LB	abbreviation of lower parameter bound
n_i	number of moles of component i
n_{ij}	number of moles of component i in phase j
N	matrix of stoichiometric coefficients
NFE	abbreviation of number of function evaluations
N_i	Krill Herd distribution
NN	herd size
n_{ref}	vector of the molar compositions in terms of the reference components
P	pressure
PE	abbreviation of phase equilibrium
PS	abbreviation of phase stability
R	universal gas constant
rand$\in[i,j]$	a randomly selected number in the range i to j.
rPE	abbreviation of reactive phase equilibrium
SC	abbreviation of stopping condition
SR	abbreviation of success rate
t	time
Δt	scaling parameter of speed vector
tol	tolerance
TPDF	tangent plane distance function
u	Lévy flight distribution
UB	abbreviation of upper parameter bound
x_i	liquid composition of component i
X_i	position of the ith krill individual
X_{best}	optimal Krill position
$\widehat{X}_{i,j}$	relative attraction between krill individuals i and j
$\widehat{X}_{i,ibset}$	relative position of the current individual, X_i to its previous best value
y_i	trial composition of component i
z_i	initial composition of component i
γ_i	activity coefficient of component i in a mixture
$\in$	tolerance of optimization
ε_i	fraction of component i in a phase
ζ_{ij}	fraction of component i in phase j
λ	Lévy flight distribution exponent
μ_i	chemical potential of component i in a mixture
μ_i^0	chemical potential of pure component i
π	total number of phases
ϕ_i	fugacity coefficient of component i
$\widehat{\phi}_i$	fugacity coefficient in solution of component i
O	the big O

Subscripts/superscripts

calculated	a calculated parameter
F	parameter evaluated at feed condition
food	parameter evaluated at food location
global	a global optima
initial	an initial guess of a parameter
T	a total parameter

factors; firstly, the number and types of phases (vapour/liquid) are not known before the optimization procedure. Secondly, the non-linearity of the various thermodynamic models usually applied to PE modelling such as cubic equations of state and complex activity coefficient models, infer local minima with objective function values very close to the global minima, especially near the critical region and phase boundaries. Furthermore, non-physical and trivial solutions are often possible at local minima. The consequences of erroneously considering local minima as the global minimum can lead to, for instance, prediction of false phase splits, as discussed by Gau et al. (2000) and Ohanomah and Thompson (1984). Thirdly, in systems exhibiting multiple phases such as vapour–liquid–liquid at equilibrium, a large difference in the Gibbs energy exists between the vapour and liquid phases, with much smaller differences in the Gibbs energy between the two liquid phases. Consequently optimization techniques struggle to locate the global minimum due to the large variance in the orders of magnitude of the terms that comprise the objective function.

Numerous global optimization methods are available in the literature (Land and Doig, 1960; Kirkpatrick et al., 1983; Dorigo, 1992; Duan et al., 1992; Hansen and Ostermeier, 2001; Mordecai, 2003; Walster and Hansen, 2004; Srinivas and Rangaiah, 2007; Yang, 2010; Yang and Deb, 2010; Walton et al., 2011; Gandomi and Alavi, 2012; Wang et al., 2013), and are generally classified as either deterministic or stochastic. Deterministic methods often require a large amount of computational time, as well as restrictions on the continuity and convexity of the objective function such as with cutting plane (Mordecai, 2003), branch and bound (Land and Doig, 1960) and interval analysis algorithms (Walster and Hansen, 2004).

Conversely the stochastic methods require very limited information on the nature of the optimization problem, and are able to handle issues pertaining to discontinuity and convexity. The computing time is generally reasonable and convergence to the global optimum is highly probable.

Metaheuristic optimization techniques are a sub category of the stochastic methods and involve an intelligent selection of random variables, often modelled around natural activities such as the cooling and heating of metal (simulated annealing, Kirkpatrick et al., 1983), the evolution of a species (differential evolution, Srinivas and Rangaiah, 2007), the swarm intelligence of insects (ant colony Dorigo, 1992, and firefly algorithms Yang, 2010), or the reproduction strategy of cuckoos (Cuckoo Search) (Walton et al., 2011; Yang and Deb, 2010). Each technique has its own strengths and weaknesses, the revision of which is beyond the scope of this work. Rashedi et al. (2009) state that, to date (2009), no single stochastic technique is capable of solving all optimization problems of different types and structures. The Krill Herd algorithm introduced by Gandomi and Alavi (2012) is a metaheuristic based on the simulation of the behaviour of a herd of the Antarctic krill crustacean,