Inverse Problems, Design and Optimization Symposium
Rio de Janeiro, Brazil, 2004

INVERSE DESIGN OF ALLOYS FOR SPECIFIED STRESS, TEMPERATURE AND TIME-TO-RUPTURE BY USING STOCHASTIC OPTIMIZATION

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ABSTRACT

The inverse problem in design of alloys is determination of chemical composition(s) of alloy(s) that will provide specified levels of, for example, stress at a specified temperature for the specified length of time. The inverse problem can be then formulated as, for example, a multi-objective optimization problem with a given set of equality constraints. This paper offers several formulations for the multiple objective functions and comparatively evaluates these models when using optimization to solve this *de facto* inverse problem.

INTRODUCTION

Our research recently concentrated on the inverse method in predicting chemical composition of steel alloys. It is a highly innovative approach that has received a warm welcome by some of the materials engineering experts from industry. For example, this formulation allows a structural design engineer who designed a machine part to ask a materials scientist to provide a precise chemical composition of an alloy that will sustain a specified stress level, at a specified temperature, and last until rupture for a specified length of time. This inverse method uses a variant of Prof. Yegorov-Egorov's optimization algorithm known as IOSO [1,2,3] to determine not one, but a number of alloys (Pareto front points) each of which will satisfy the specified properties while having different percentages of each of the alloying elements (a different "recipe"). This provides the user of the alloy with increased flexibility when deciding to create such an alloy, because he/she can use the "recipe" which is made of the most readily available and the most inexpensive elements on the market at that point in time.

We have developed several mathematical formulations and corresponding software packages for different ways how to achieve inverse determination of chemical compositions of alloys that simultaneously satisfy several specified mechanical and cost/availability properties. These different formulations were then compared and analytically evaluated in an attempt to determine the most appropriate formulation. This way, the customer can choose the optimized alloy composition that is the most available and the least expensive at a moment when it is ordered from the alloy manufacturer.

It should be pointed out that inverse problem of determining alloy chemical composition is different from a direct optimization problem [4,5,6] of designing alloys that will have extreme properties.

FORMULATIONS

In particular, the objective was to determine chemical composition(s) of high temperature steel alloys that will have specified (desired) physical properties. Design variables were concentrations (percentages) of each of the following 14 alloying elements ***C, S, P, Cr, Ni, Mn, Si, Mo, Co, Cb, W, Sn, Zn, Ti***

No mathematical analysis was used to evaluate the objectives. The evaluations were performed using classical experiments on candidate alloys. In other words, we used an existing experimental database [4,5,6]. Optimization criteria was formulated as a multi-objective statement with three simultaneous objectives: minimize the difference between the specified and the actual stress, minimize the difference between the specified and actual maximum temperature, and minimize the difference between the specified and actual time to rupture (Table 1).

Table 1. Eight formulations for objective functions and constraints

		Objectives (minimize)				Constraints (minimize)
Model number	**Number of objectives**	**Stress**	**Operating temperature**	**Time until rupture**	**Low cost alloy**	
1	3	$(\sigma-\sigma_{spec})^2$	$(T-T_{spec})^2$	$(\theta-\theta_{spec})^2$		
2	1	$(\sigma-\sigma_{spec})^2+(T-T_{spec})^2+(\theta-\theta_{spec})^2$				
3	3	$(\sigma-\sigma_{spec})^2$	$(T-T_{spec})^2$	$(\theta-\theta_{spec})^2$		$(\sigma-\sigma_{spec})<\varepsilon$ $(T-T_{spec})<\varepsilon$ $(\theta-\theta_{spec})<\varepsilon$
4	1	$(\sigma-\sigma_{spec})^2+(T-T_{spec})^2+(\theta-\theta_{spec})^2$				$(\sigma-\sigma_{spec})<\varepsilon$ $(T-T_{spec})<\varepsilon$ $(\theta-\theta_{spec})<\varepsilon$
5	1	$(\sigma-\sigma_{spec})^2$				$(T-T_{spec})<\varepsilon$ $(\theta-\theta_{spec})<\varepsilon$
6	1		$(T-T_{spec})^2$			$(\sigma-\sigma_{spec})<\varepsilon$ $(\theta-\theta_{spec})<\varepsilon$
7	1			$(\theta-\theta_{spec})^2$		$(\sigma-\sigma_{spec})<\varepsilon$ $(T-T_{spec})<\varepsilon$
8	10	$(\sigma-\sigma_{spec})^2$	$(T-T_{spec})^2$	$(\theta-\theta_{spec})^2$	Ni, Cr, Nb, Co, Cb, W, Ti	

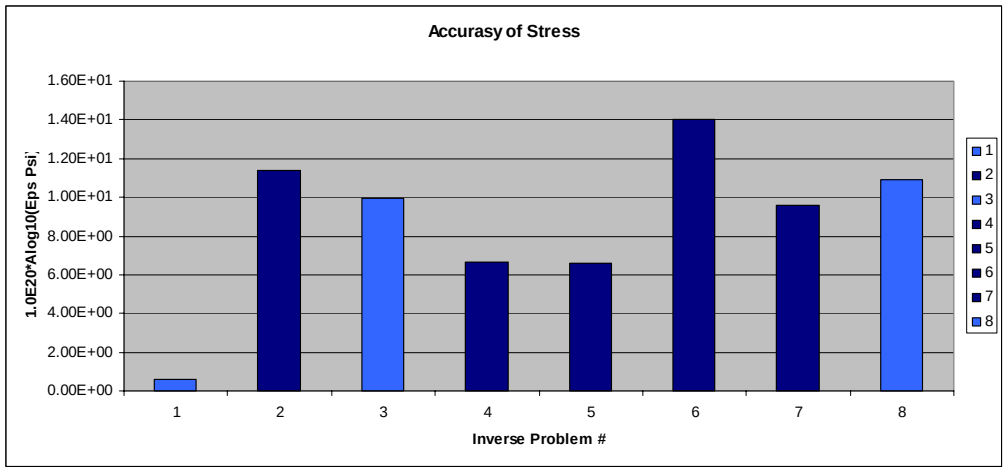

Fig. 1 Accuracy of satisfying the specified stress for eight formulations

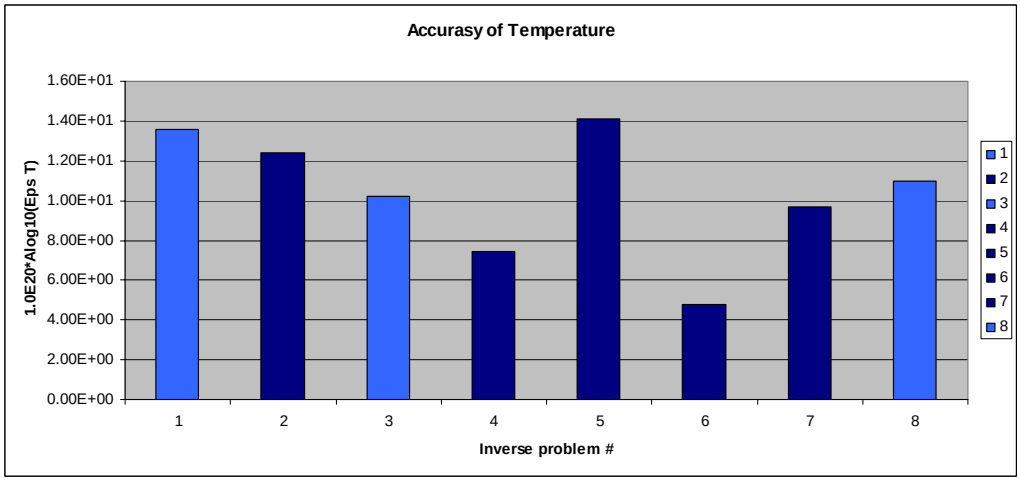

Fig. 2 Accuracy of satisfying the specified temperature for eight formulations

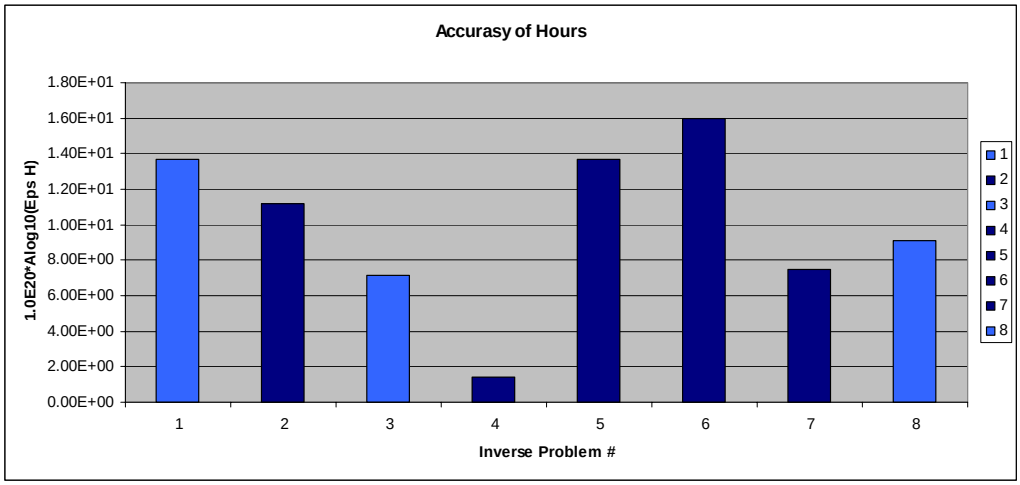

Fig. 3 Accuracy of satisfying the specified time-to-rupture for eight formulations

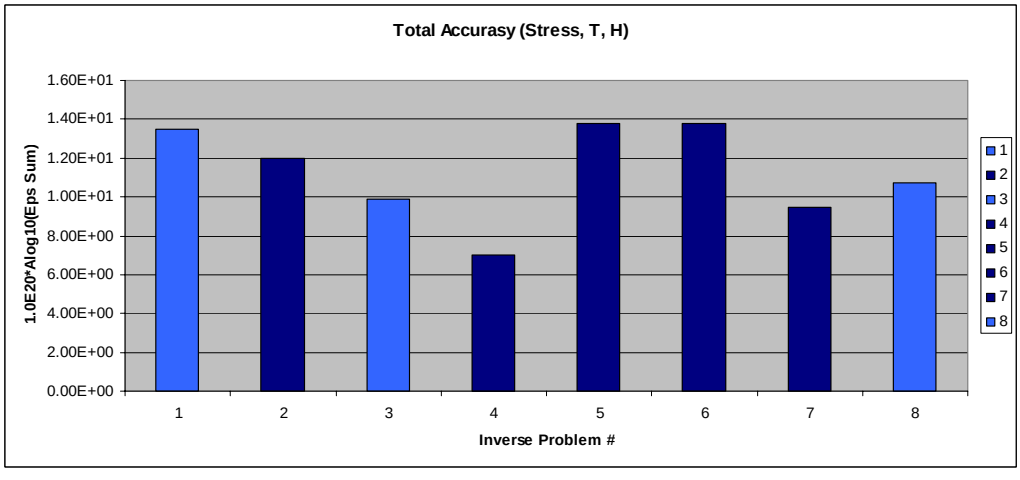

Fig. 4 Combined accuracy of satisfying the specified values for eight formulations

$$\Delta\sigma = \left(\sigma - \sigma_{spec}\right)/\sigma_{spec}, \quad \Delta T = \left(T - T_{spec}\right)/T_{spec}, \quad \Delta\theta = \left(\theta - \theta_{spec}\right)/\theta_{spec}$$

$$K_1 = 10\,N_{objectives} + N_{constraints} + N_{variables} \qquad K_2 = 100\,\Delta\sigma + \Delta T + \Delta\theta \qquad K_3 = N_{calls}\,/\,N_{Pareto}$$

$$\text{EPS} = \sum\ 1/[\left(\sigma - \sigma_{spec}\right)^2 + \left(T - T_{spec}\right)^2 + \left(\theta - \theta_{spec}\right)^2]$$

Maximize: $SCORE = K_1 K_2 \exp(EPS)/K_3$

Fig. 5 An ad hoc analytical formulation for the overall performance evaluation of the various inverse design formulations

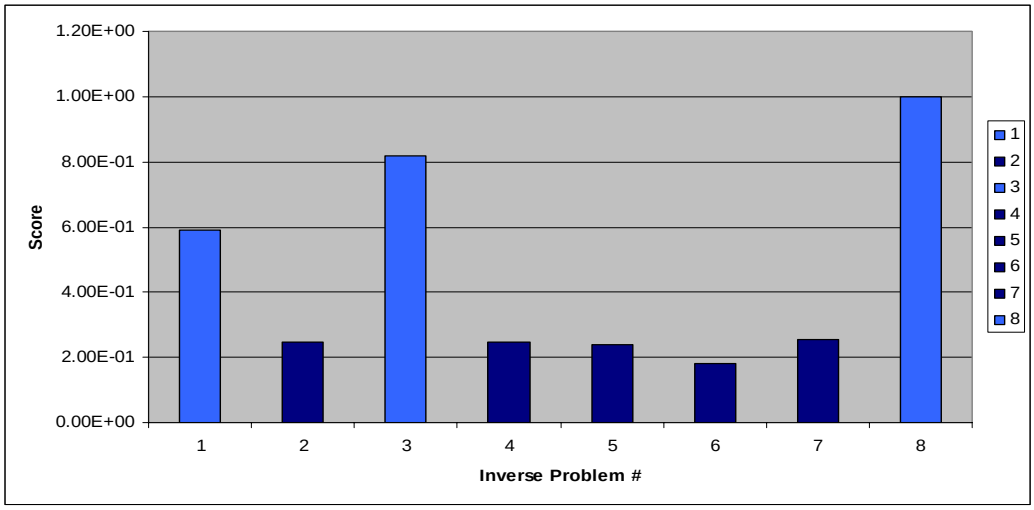

Fig. 6 Comparison of overall performance of the eight inverse formulations

	Eps_{str}	Eps_{t}	Eps_{h}	Eps_{sum}	N_{Const}	N_{Obj}	$N_{Points\ (Pareto)}$	N_{Calls}	Score
Prob. 1	.408E-19	.356E-06	.536E-06	.297E-06	0	3	50	417	0.590
Prob. 2	.269E-08	.267E-07	.172E-08	.104E-07	3	1	1	703	0.246
Prob. 3	.897E-10	.143E-09	.134E-12	.777E-10	3	3	50	445	0.817
Prob. 4	.434E-13	.289E-12	.244E-18	.111E-12	3	1	1	1020	0.246
Prob. 5	.413E-13	.139E-05	.549E-06	.646E-06	2	1	1	601	0.239
Prob. 6	.954E-06	.576E-15	.980E-04	.646E-06	2	1	1	774	0.180
Prob. 7	.408E-10	.515E-10	.299E-12	.309E-10	2	1	1	776	0.256
Prob. 8	.714E-09	.928E-09	.127E-10	.552E-09	3	10	46	834	1.000

Fig. 7 Summary of accuracies in satisfying objectives, number of constraints, number of simultaneous objectives, number of Pareto points generated, number of optimization algorithm calls required, and the final performance scores of the eight formulations

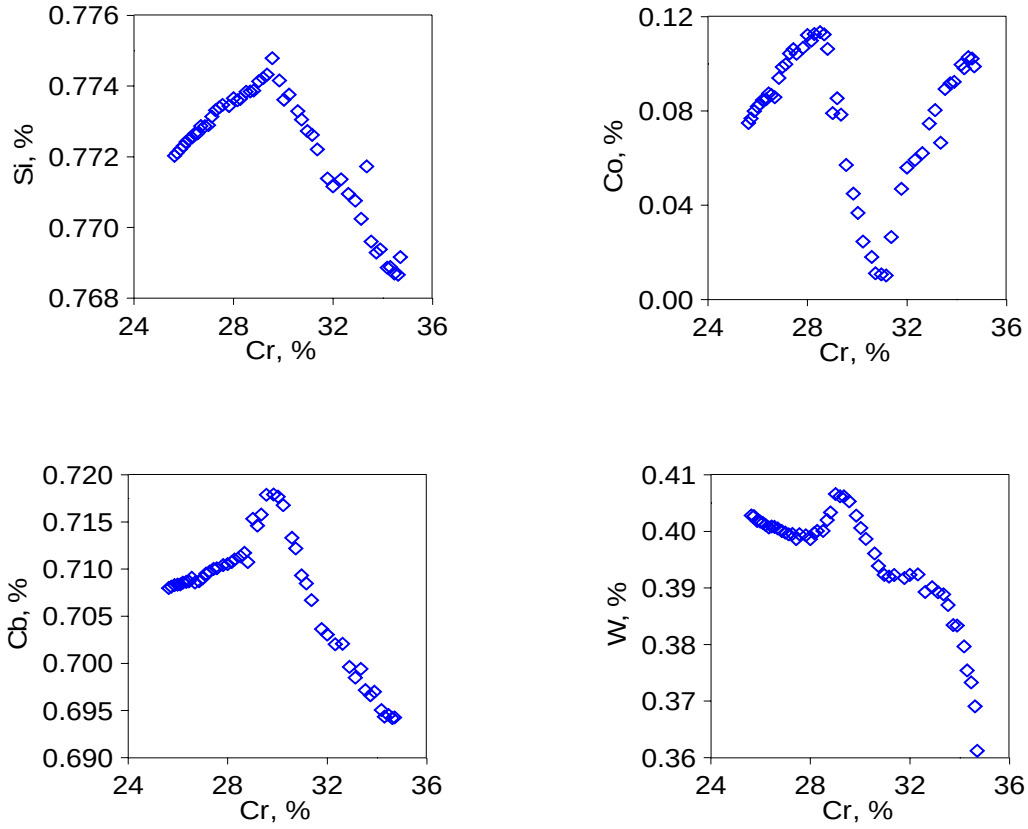

Fig. 8 Allowable variations of concentrations of several alloying elements with respect to Cr when specifying stress (230 N mm^{-2}), temperature (975 C) and time-to-rupture (5000 hours)

RESULTS

In the case of inversely determining concentrations of each of the 14 chemical species in steel alloys when using the eight mathematical formulations for the objective function(s) and constraints (Table 1), it is apparent that IOSO optimization algorithm offers consistently high accuracy in satisfying the specified stress (Fig. 1), operating temperature (Fig. 2), time-to-rupture (Fig. 3) and an overall combined accuracy (Fig. 4). When the suggested eight formulations were evaluated using an *ad hoc* evaluation procedure (Fig. 5), only a few formulations appear to offer an overall superior performance (Figs. 6 and 7). The predicted combinations of concentrations of alloying elements vary rapidly (Fig. 8) suggesting that only robust non-gradient based optimization algorithms could handle these types of problems.

This methodology of inversely designing chemical compositions of alloys offers a significant freedom to the designer to choose from a relatively large number of possible chemical compositions that satisfy the same specified physical properties.

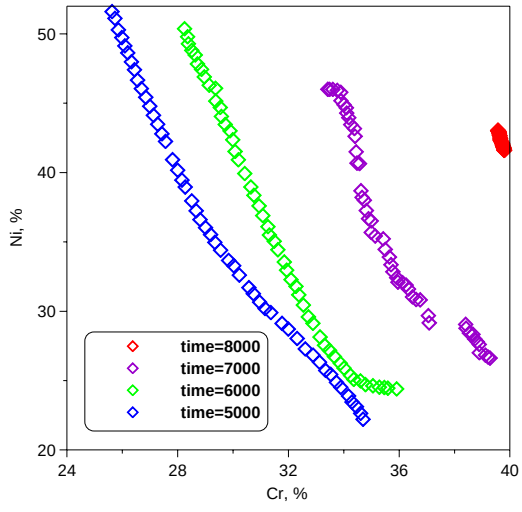

Fig. 9 Allowable ranges of Ni and Cr concentrations for a specified level of stress and temperature and different life expectancies.

For example, if the designer specifies the desired stress level of 230 N mm^{-2} and the desired temperature of 975 C, there will be 50 possible combinations of Ni and Cr concentrations that will all provide life expectancy of 5000 hours. If the life expectancy is specified by the designer to be 6000 hours for the same stress and temperature levels, the allowable range of possible combinations of Ni and Cr concentrations will decrease. This will become increasingly more noticeable as the specified life expectancy is increased further to 7000 and eventually to 8000 hours (Fig. 9).

The results of this multiple simultaneous least-square constrained minimization problem cannot be visualized for more that two alloying species at a time. For example, when concentrations of only two alloying elements like Ni and Cr are visualized, and temperature and life expectancy are unconstrained (unspecified) the optimizer will give a fairly large domain for possible variations of the concentrations of Cr and Ni. But, as the constraints on temperature level are introduced and progressively increased, the feasible domain for varying Cr and Ni will start to shrink (Fig. 10). Similar general trend can be observed when the life expectancy is specified and progressively increased.

Finally, when temperature level and the life expectancy are prescribed simultaneously and progressively increased simultaneously, the feasible domain for concentrations of Cr and Ni reduces rapidly (Fig. 11). Similar trends could be observed when looking at any other pair of alloying elements.

CONCLUSIONS

A new concept has been developed for designing alloys having specified multiple physical properties. This inverse problem was formulated as a constrained multi-objective optimization problem and solved using a robust evolutionary optimizer of IOSO type. As a result, multiple choices are obtained for combinations of concentrations of alloying elements whereby each of the combinations corresponds to another Pareto front point and satisfies the specified physical properties. This alloy design methodology does not require knowledge of metallurgy or crystallography and is directly applicable to alloys having arbitrary number of alloying elements.

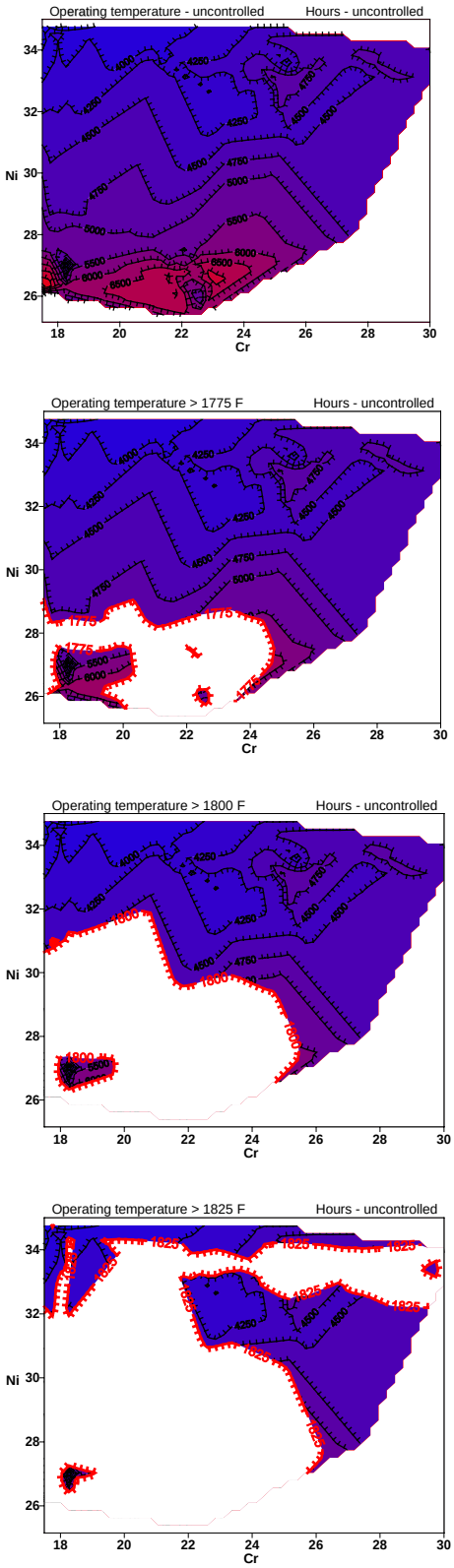

Fig. 10 Effect of increasing the temperature

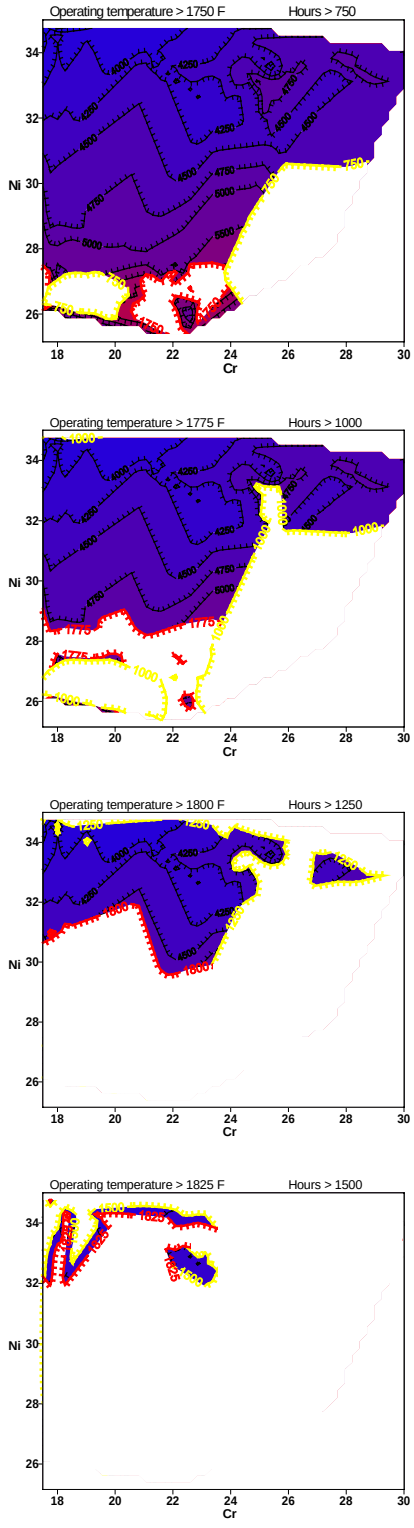

Fig. 11 Efect of simultaneously increasing temperature and life expectancy

ACKNOWLEDGEMENTS

The authors are grateful for the financial support provided for this work by the US Department of Energy under the grant DE-FC07-01ID14252 and by the US Army Research Office under the grant DAAD 19-02-1-0363 monitored by Dr. W. Mullins.

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