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Editors' Remarks

THE GOLDEN APPLES OF THE SUN

'South', said the captain.
'But', said his crew, 'there simply aren't any directions out here in space.'
'When you travel on down toward the sun,' replied the captain, 'and everything gets yellow and warm and lazy, then you're going in one direction only.' He shut his eyes and thought about the smoldering, warm, faraway land, his breath moving gently in his mouth. 'South.' He nodded slowly to himself. 'South.'
Their rocket was the *Copa de Oro*, also named the *Prometheus* and the *Icarus*, and their destination in all reality was the blazing noonday sun. In high good spirits they had packed along two thousand sour lemonade: and a thousand white-capped beers for this journey to the wide Sahara. And now as the sun boiled up at them they remembered a score of verses and quotations:
'The golden apples of the sun?'
'Yeats'.
'Tear no more the heat of the sun?'
'Shakespeare, of course'
'Cop of Gold'? Steinbeck, 'The Crock of Gold?' Stephens.
And what about the pot of gold at die rain-bow's end?
There's a name for our trajectory, by God. 'Rainbow!'
'Temperature?'
'One thousand degrees Fahrenheit!'

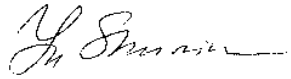
Ray Bradbury,
'The Golden Apples of the Sun'
from 'The Golden Apples of the Sun'

This 13th volume No.1 is devoted to various questions of **solid state physics** and **applied statistics**. In particular, we present actual papers from Israel, Ukraine, Byelorussia, Lithuania and Latvia.

Our journal policy is directed on the fundamental and applied sciences researches, which are the basement of a full-scale modelling in practice.

This edition is the continuation of our publishing activities. We hope our journal will be interesting for research community, and we are open for collaboration both in research and publishing. This number opens the current 2009 year of our publishing work. We hope that journal's contributors will consider the collaboration with the Editorial Board as useful and constructive.

EDITORS



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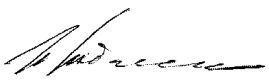

I.V. Kabashkin

Computer Modelling and New Technologies, 2009, Vol.13, No.1, 7–16
Transport and Telecommunication Institute, Lomonosova 1, LV-1019, Riga, Latvia

ELECTRONIC STRUCTURE AND CHEMICAL BONDING IN LAVES PHASES Al_2Ca, Be_2Ag AND Be_2Ti

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The results of *ab-initio* calculations of electronic structure of Laves-phase compounds Al_2Ca, Be_2Ag and Be_2Ti are presented. Calculations were carried out in the framework of Density Functional Theory (DFT) and the Full Potential Linearized Augmented Plane Waves + local orbital formalism (FP APW+lo). Total, local and partial densities of electronic states (DOS) were obtained and analysed. These data together with differential electronic density (DED) distribution allow understanding the links of chemical bonding with structural stability of studied compounds.

Keywords: *Laves-phases, ab initio calculations, chemical bonding*

1. Introduction

Laves phases, with a composition AB_2, are intermetallic compounds generally crystallized into three close-packed structures: cubic (C15-$MgCu_2$), hexagonal (C14-$MgZn_2$) and di-hexagonal (C36-$MgNi_2$) [1, 2].

Last time Laves-phase compounds have been widely investigated due to new perspectives of their applications. For example, $CeRu_2$ and (Hf, Zr)V_2 compounds are known as super conducting materials [3, 4]. (Tb, Dy)Fe_2 compound reveals a giant magneto-striction [5]. (Ho, Mm)Co_2 compound can be used as hydrogen storage reservoir [6]. Compounds $NbCr_2$ and HfV_2 attract an interest due to their hardness to high temperatures [7, 8].

Laves-phase crystals are typical size factor compounds with an atomic size ratio R_A/R_B around 1.225 (where R_A and R_B are diameters of A and B atoms, respectively [9]). Their stability depends strongly on electronic structure of constituent atoms. Detailed information regarding the nature of chemical bonds allows understanding physical and chemical properties of Laves phases. In [10] calculations of densities of states and charge density distribution in $TiCr_2$ were reported. A large covalent component in bonding of small atoms (Cr) was found. In [11] an electronic structure of paramagnetic Laves phases HfV_2 and $HfFe_2$ was calculated using FP APW + lo formalism. A significant overlap of wave functions for the neighbouring V-V and Fe-Fe atoms shows their mainly covalent bonding. *Ab initio* calculations of electronic structure of Al_2Ca, Al_4Ca and Mg_2Ca phases [12] showed that among these compounds Al_2Ca phase has the strongest alloying ability and the highest structural stability.

We report results of *ab initio* calculations of electronic structure of three Laves-phase compounds: Al_2Ca, Be_2Ag and Be_2Ti. Unlike Al_2Ca, in Be_2Ag and Be_2Ti compounds the constituent atoms (Ag and Ti) contain *d*-electrons that participate in formation of chemical bonds. It is shown that a structural stability of studied compounds depends on participation of electrons of different symmetry in chemical bonding.

2. Methodology of Calculations

The calculations are carried out in the framework of DFT [13, 14] and FP LAPW + lo formalism [15, 16]. Within this method, the unit cell is divided into two regions in a manner reminiscent of a muffin tin (*mt*) spheres. The first region consists of non-overlapping spheres (with radii R_{mt}) around each atomic centre. In this region, the Kohn-Sham wave functions are taken as atomic-like functions (Eq. 1), which are solutions for a spherical potential. The second region is the remaining space outside the *mt* spheres, so called the interstitial region (*IR*). In *IR* electrons are described by plane waves (Eq. 2).

$$\Phi_{\vec{k}_n}(\vec{r}) = \sum_{lm} A_{lm,\vec{k}_n} u_l\left(\vec{r}, E_l\right) Y_{lm}\left(\hat{r}\right) + \varphi_{\text{lo}},\ \vec{r} \in \text{atomic sphere}, \tag{1}$$

$$\Phi_{\vec{k}_n}(\vec{r}) = \frac{1}{\sqrt{\omega}} e^{i\vec{k}_n \cdot \vec{r}},\ r \in \text{ interstitial region}. \tag{2}$$

Here A_{lm} are coefficients, $\vec{k}$ is the wave vector inside the first Brillouin zone, $\vec{k}_n = \vec{k} + \vec{K}_n$ where $\vec{K}_n$ is a reciprocal lattice vector, ω is a normalizing volume per atom. $u_l(\vec{r}, E_l)$ is a regular solution of the radial part of Schrödinger equation for energy E_l. Y_{lm} are spherical harmonic functions, l and m are angular momentum quantum numbers. φ_{lo} is the wave function of a local orbital. The solution of the Kohn-Sham equations is expended in this combined basis set of functions according to the linear variation method, $\Psi_{\vec{k}}(\vec{r}) = \sum_n c_n \Phi_{\vec{k}_n}(\vec{r})$ where coefficients c_n are determined by the Rayleigh-Ritz variation principle.

In this work the WIEN2K package [17] was used. The core states are treated in fully relativistic approximation [18] while the valence states are treated in a scalar relativistic approximation [19]. The exchange-correlation potential within the Perdew-Burke-Ernzerhof (PBE) generalized gradient approximation (GGA) [20] was used. The calculations are performed within the spin-polarization approximation.

To find the equilibrium lattice parameters of studied phases the total energy was optimised by variation of the volume per atom. The accuracy of the total energy self-consistent calculations is ~10^{-4} Ry. In the framework of FP LAPW + lo method the *mt* spheres should not overlap. On one hand, the increasing R_{mt} significantly decreases the computation time. On the other hand, too large R_{mt} can lead to the overlapping of *mt* spheres when the lattice parameter becomes small in the optimisation procedure. To satisfy these conditions we have chosen $R_{mt} = 2$ a.u. for all atoms in all calculations. To achieve the required accuracy in the total energy calculations two additional input parameters in the program should be determined. One of them is the number of *k*-points in the first Brillouin zone. It provides the accuracy of the summation over *k* in the first Brillouin zone. Another one is the number of plane waves in the expansion of the wave functions in the interstitial region, which is determined by K_{max}. It was found that for the phase Al_2Ca a *k*-mesh of about 1000 points in the first Brillouin zone makes the total energy independent on the number of *k*-points with the required accuracy, while for Be_2Ag and Be_2Ti a *k*-mesh of 1500 points satisfies this condition (see example on Fig. 1.). The magnitude of $R_{mt}K_{max}$ that gives an accuracy of the total energy calculations ~10^{-4} Ry was equal to 8.5 for Al_2Ca and 9 for Be_2Ag and Be_2Ti, as justified by results of calculations displayed on Figure 2, where the results for Be_2Ag are shown as the example.

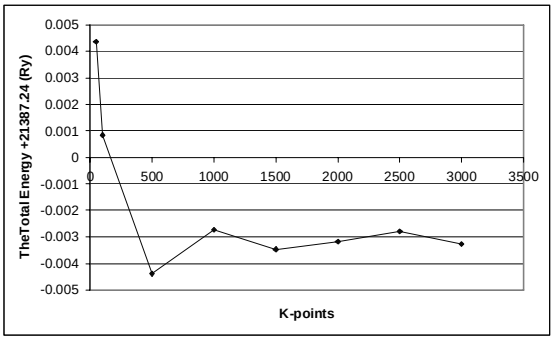


Figure 1. Total energy as a function of number of *k*-points for Be_2Ag

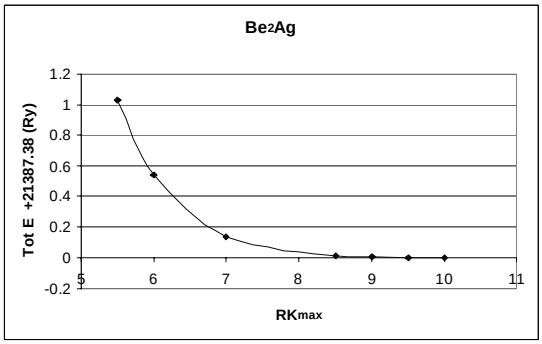


Figure 2. Dependence of the total energy on the plane-wave cut-off parameter for Be_2Ag

The energy cut-off, separating core and valence states was equal to – 6.0 Ry. This condition allowed minimizing a leak of the electron core states into interstitial region. Additional details concerning the calculation method can be found in [21].

3. Results and Discussion

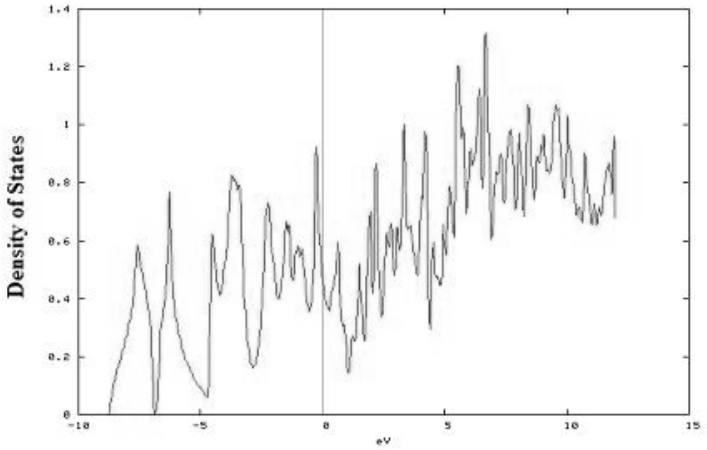
The equilibrium lattice parameters for studied Laves phases are in good agreement with experimental data published in [22] (Table 1). The calculated band structures for these compounds show that all three phases are conductive materials.

Table 1. Calculated and experimental lattice constants for considered phases (in Å)

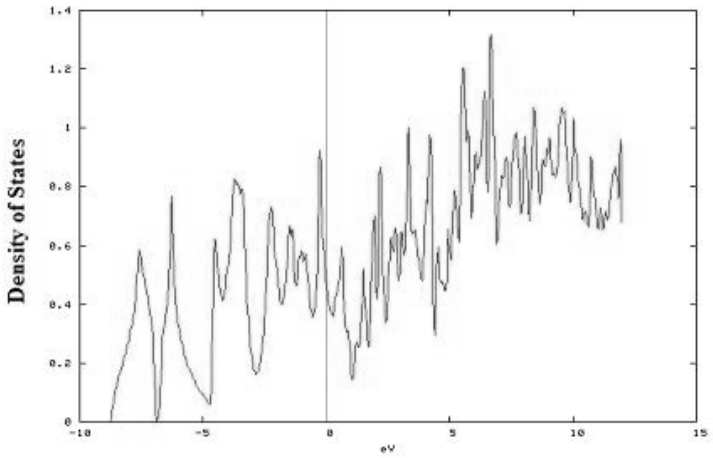
Phase	Calculated	Experiment [17]
Al_2Ca	8.02	8.02
Be_2Ag	6.44	6.43
Be_2Ti	6.29	6.407

To obtain the information about the influence of electronic properties of constitutional atoms on their chemical bonding we calculated total and partial Densities of States (DOS) for all studied phases. We proceed from the fact that electrons with energies in the region of Fermi energy, E_F play the main role in formation of chemical bonds. Comparing the total DOS for Al_2Ca (Fig. 3a) and local DOS for Al (Fig. 3b) and Ca (Fig. 3c) we conclude that electrons of Al give the main contribution to conductivity of Al_2Ca compound and accordingly cause a metallic bonding.

(a)



(b)



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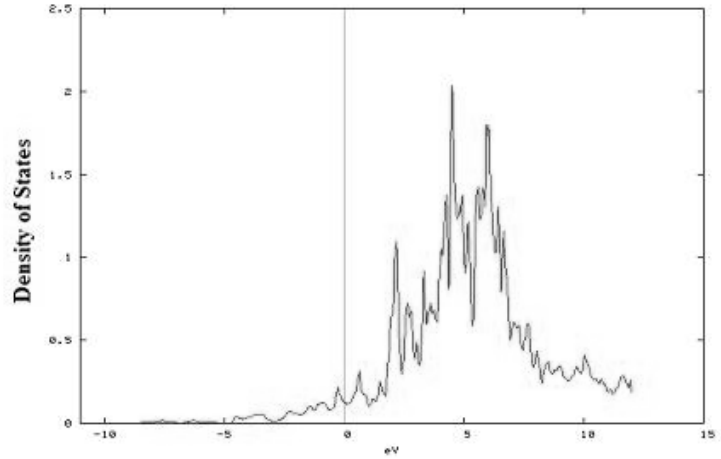
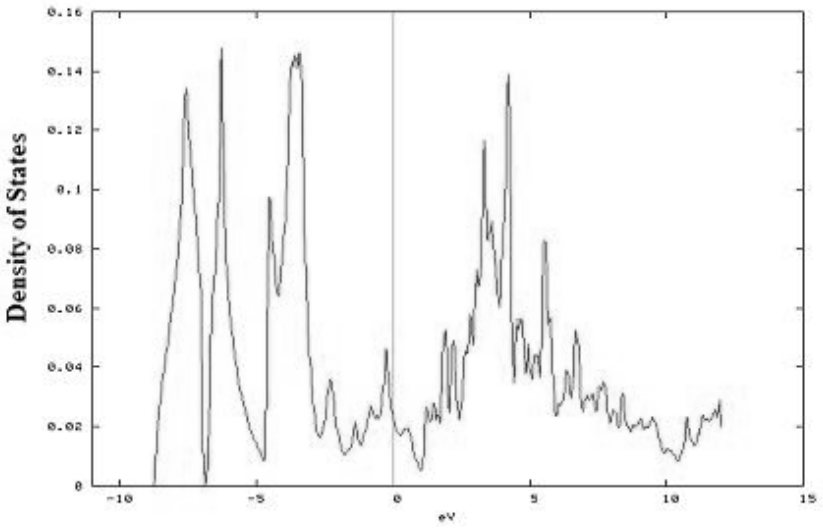
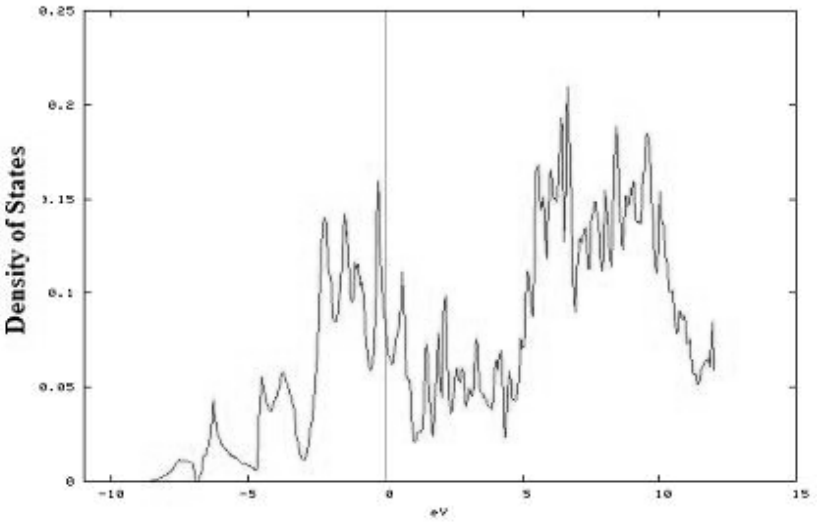


Figure 3. The total and local DOS (in states/ eV) for Al_2Ca: (a) total DOS; (b) DOS for Al atoms; (c) DOS for Ca atoms.
The zero on the x axis here and in the following Figs. corresponds to Fermi energy, E_F

(a)



(b)



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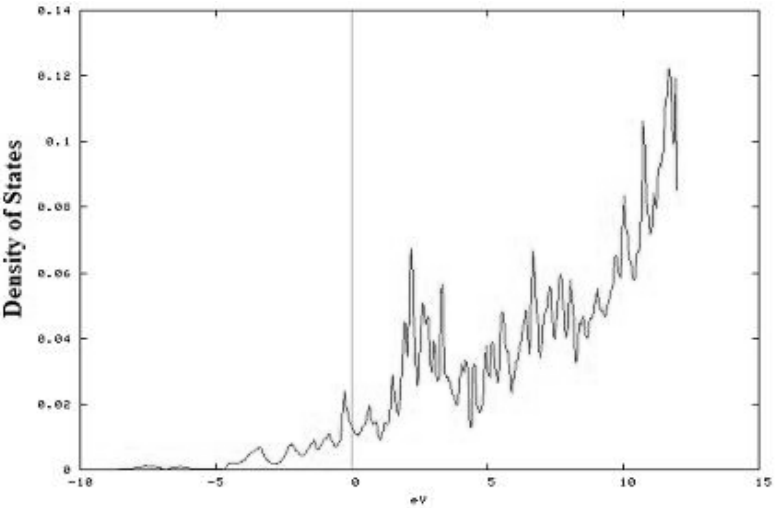


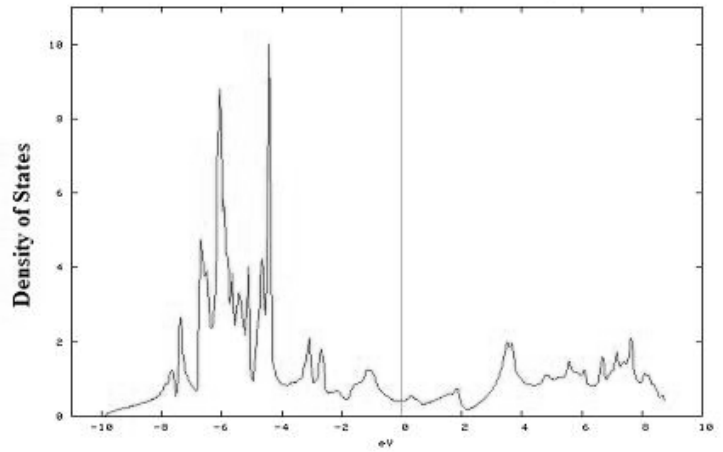
Figure 4. The partial DOS (in states/ eV) for Al_2Ca: (a) *s*-states of Al atoms; (b) *p*- states of Al atoms; (c) promoted *d*- states for electrons of Al atoms

Partial DOS for Al and Ca displayed on Figure 4 show that *s*- and *p*-electrons of Al dominate in the energy range $E \le E_F$. These results indicate that *s*- and *p*-electrons of Al determine the bonding

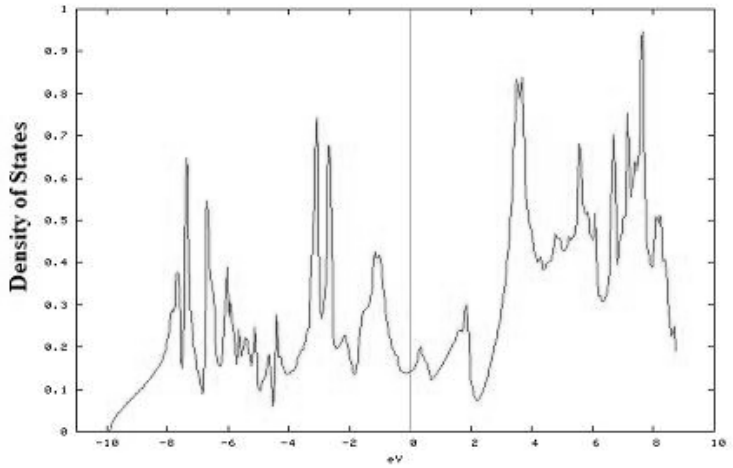
in Al_2Ca. From Figure 4c one can see that promoted *d*-electrons of Al also participate in chemical bonding. A hybridisation of *s*- *p*- and promoted *d*-electrons of Al should lead to covalent bonding in Al_2Ca but the covalent component is relatively small.

On Figures 5, 6 the results of calculations of DOS for Be_2Ag phase are presented. Comparing the total DOS for Be_2Ag (Fig. 5a) with local DOS for constitutional atoms Be (Fig. 5b) and Ag (Fig. 5c) in the energy range $E \le E_F$ it may be seen that Be atoms give a larger contribution to total DOS in comparison with Ag atoms.

(a)



(b)



(c)

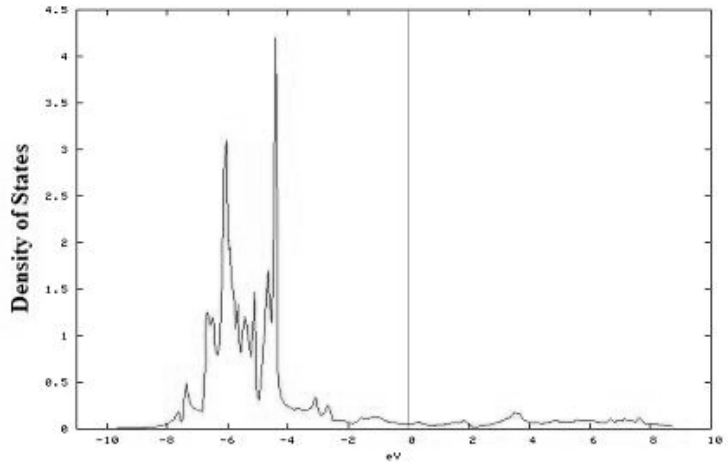


Figure 5. The total and local DOS (spin- up states) (in states/ eV) for Be_2Ag: (a) total DOS; (b) DOS for Be atoms; (c) DOS for Ag atoms

(a)

(b)

(c)

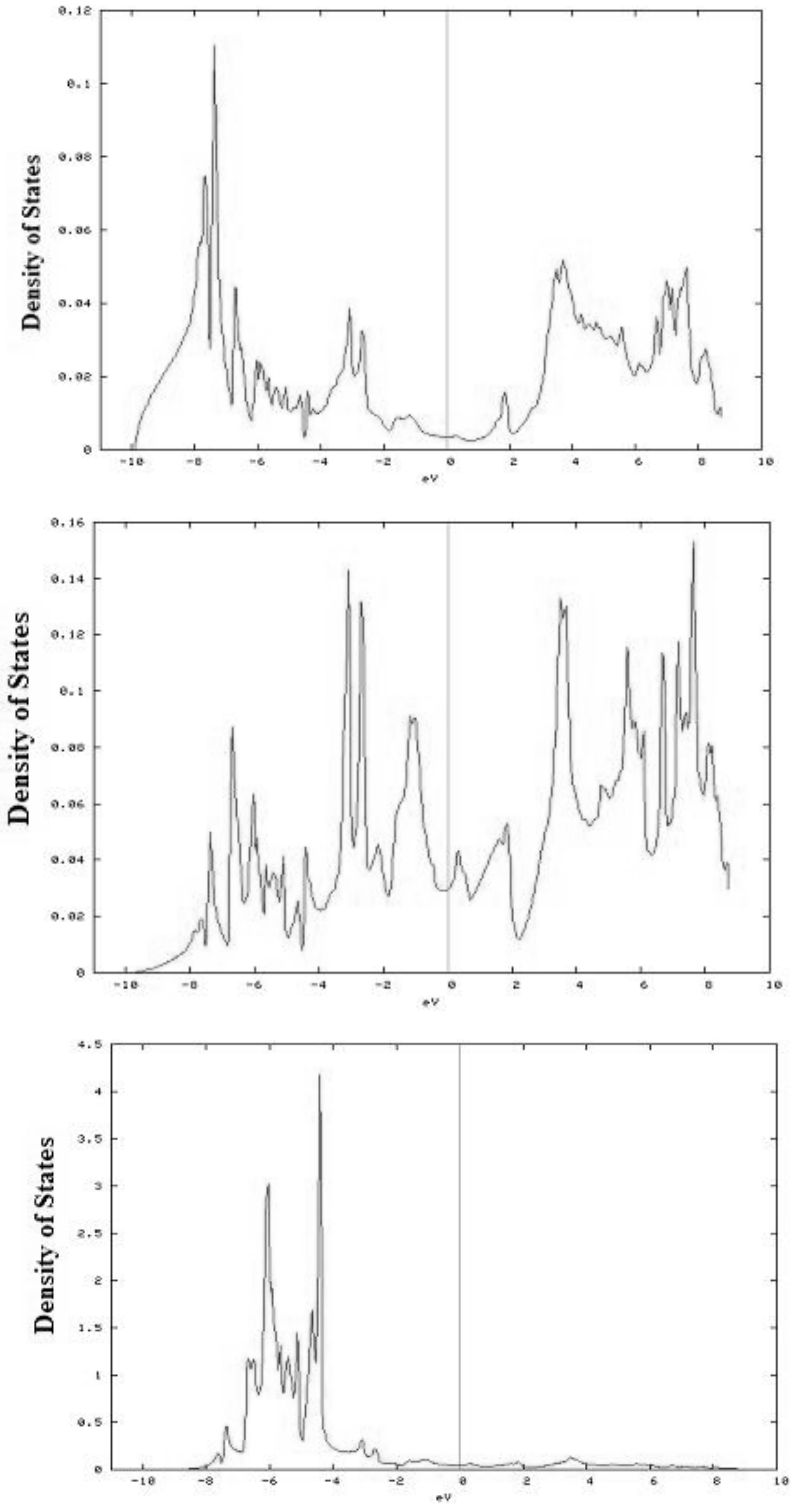
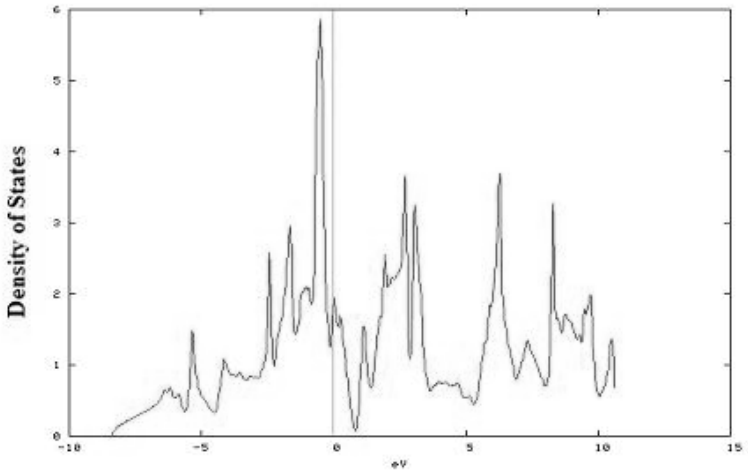


Figure 6. The partial DOS (spin-up states) (in states/ eV) for Be_2Ag: (a) s-states of Be atoms; (b) promoted *p*- states of Be atoms; (c) *d*- states of Ag atoms

Partial DOS show the formation of the promoted *p*-states for electrons of Be atoms (Fig. 6b). Hybridization is expected in the range 2–8 eV below E_F between *p*-states and *s*-states of Be (Fig. 6a and 6b) and *d*-states of Ag (Fig. 6c). A covalent component should give a visible contribution to chemical bonding. It is larger than in the case of Al_2Ca compound. A small value of total DOS at the Fermi level (Fig. 5a) shows a relatively weak metallic component in chemical bonding in the Be_2Ag phase as compared with Al_2Ca.

Analysis of DOS for Be_2Ti compound (Figs. 7 and 8) shows an overlapping of *d*-states of Ti (Figs. 8b and 8c) with promoted *p*-states of Be electrons (Fig. 8a) in the range from E_F to ~ 3eV below Fermi energy.

(a)



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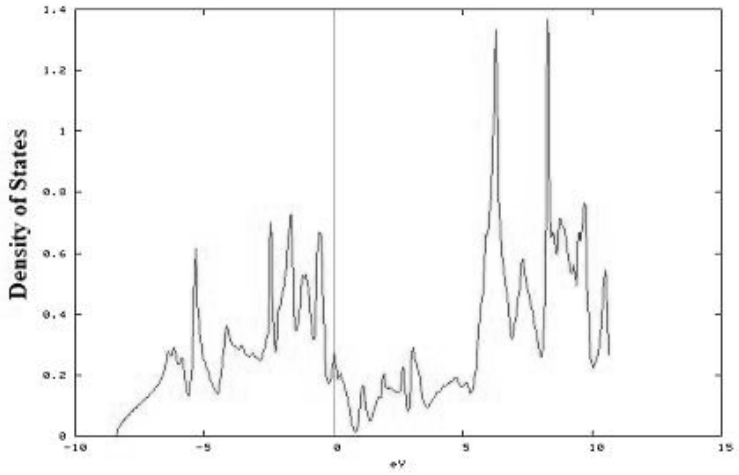

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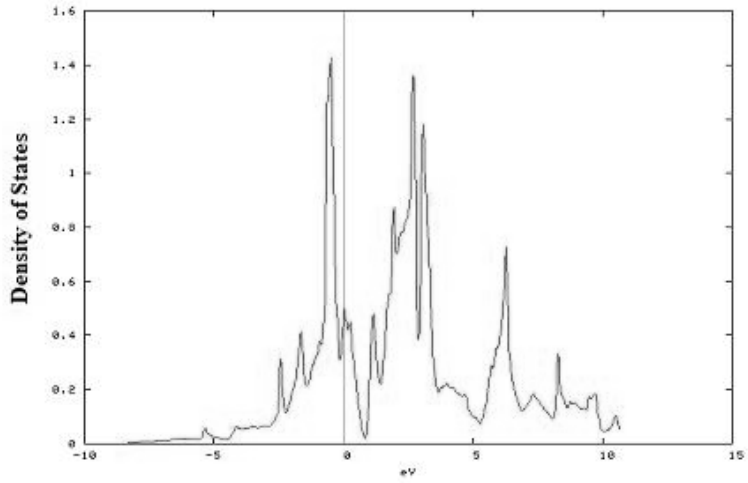

Figure 7. The total and local DOS (spin-up states) (in states/ eV) for Be_2Ti: (a) total DOS; (b) DOS for Be atoms; (c) DOS for Ti atoms

(a)

(b)

(c)

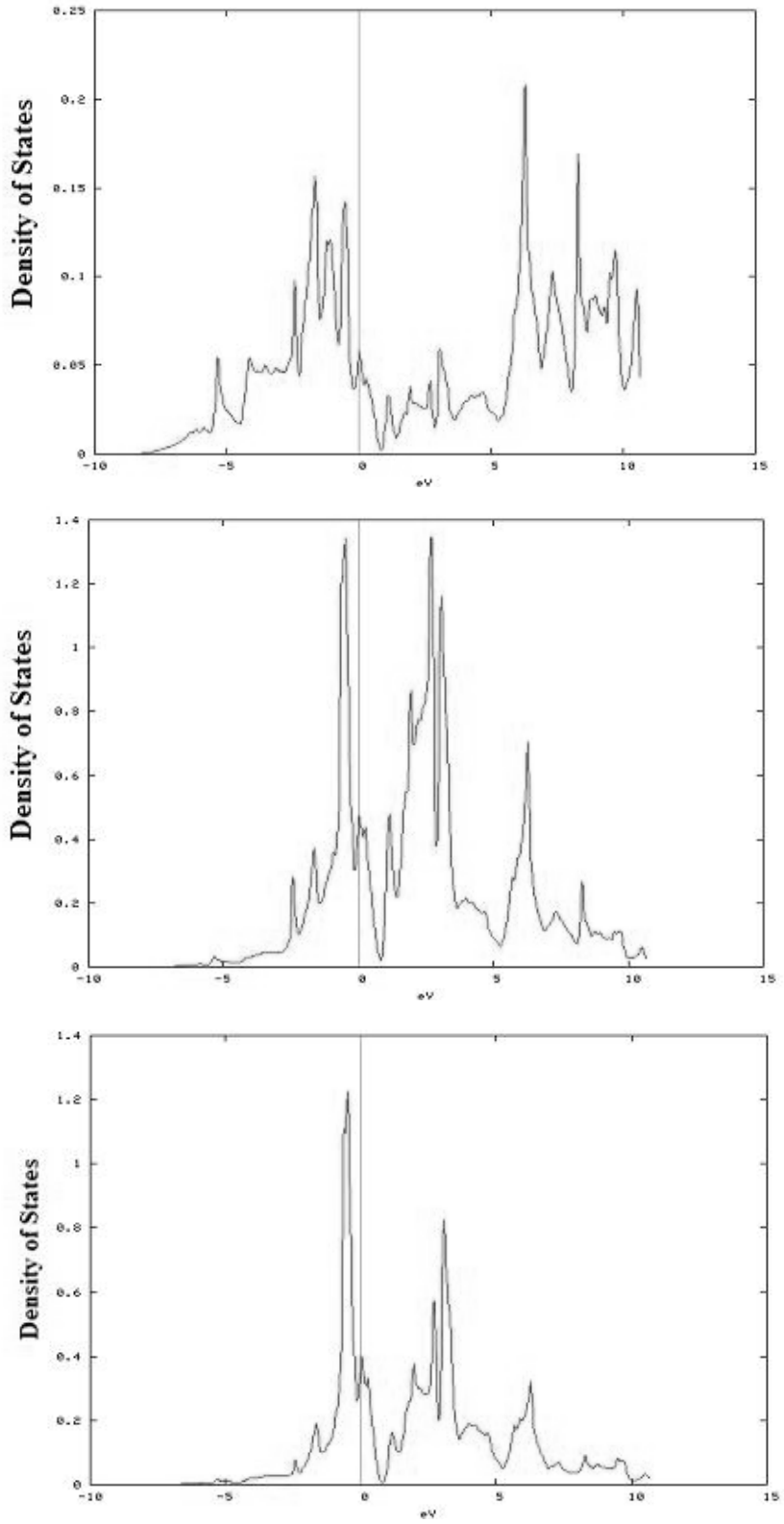

Figure 8. The partial DOS (spin-up states) (in states/ eV) for Be_2Ti: (a) promoted *p*-states of Be atoms; (b) *d*- states of Ti atoms; (c) *d*- states with t_{2g}-symmetry of Ti atoms

Conductivity in Be_2Ti phase should be higher than in Be_2Ag due to larger number of states at Fermi level (Figs. 5a and 7a). This is caused by significant contribution of *d*-electrons of Ti. The splitting of bonding and anti-bonding *d*-states of Ti located in the energy region between – 5eV and + 5ev

is clearly seen. At the same time, in Be_2Ag *d*-states of Ag are mainly located below E_F. As well as in Be_2Ag, in Be_2Ti the promoted *p*-electrons of Be form hybrid covalent bonds with *d*-electrons of Ti.

On Figure 9 the calculated Differential Electron Density (DED) in the plane (110) for studied Laves phases is presented.

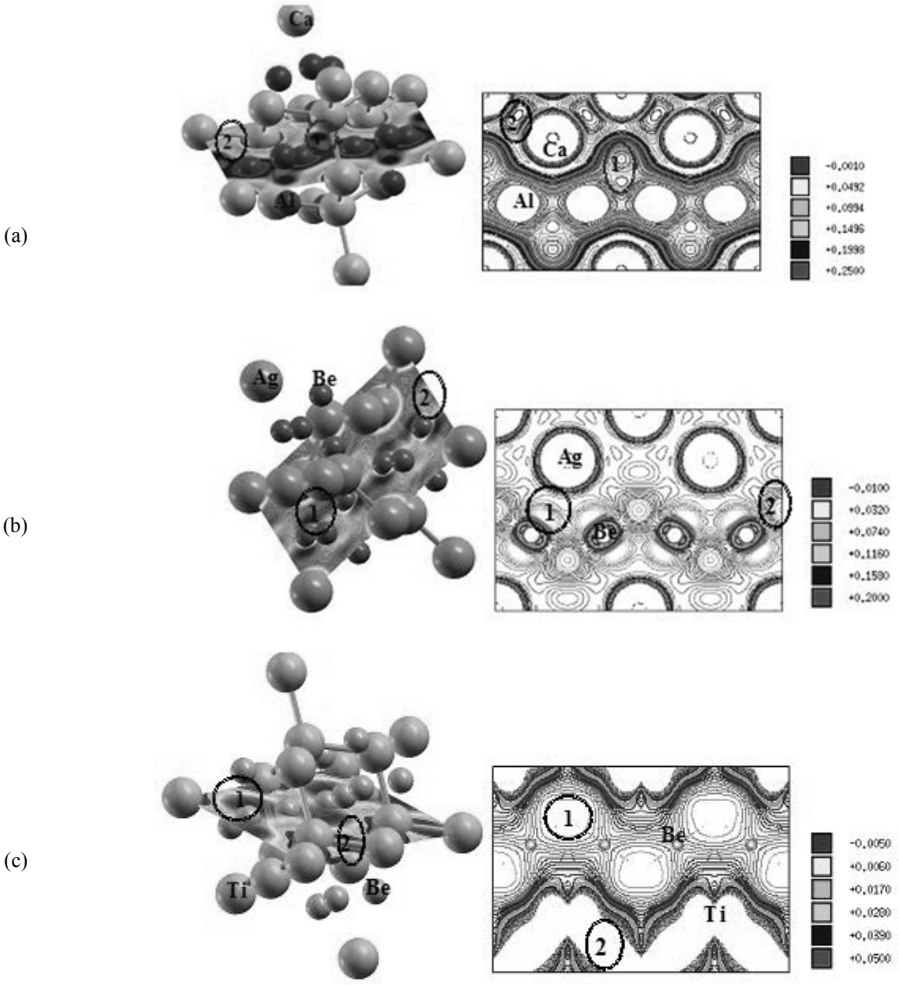

Figure 9. Mapping of spatial distributions of DED (in e/Å^3) in the plane (110) for Al_2Ca (a), Be_2Ag (b), and Be_2Ti (c)

DED shows the difference between the self-consistently calculated electron density in the phases and the sum of the atomic electron densities. Peculiarities of spatial DED distribution can be understood on the basis of described DOS analysis. The regions of the relative lack of DED and of the extra electron charge are seen. For example, let us consider the peculiarities of DED behaviour for Al_2Ca. In region 1 (Fig. 9.a) we obtained the value of DED equal to + 0.1998 e/Å^3. The values of DED in this region are mainly caused by the redistribution of the electrons that belong to Al atoms that are placed above and beneath the plane (110). In region 2 the value of DED (+ 0.0944 e/Å^3) is mostly caused by atoms surrounding Ca. It is lower in comparison with the value of DED in region 1 that is explained by the degree of overlapping of electronic orbits of constitutional atoms discussed above.

For the phase Be_2Ag in the plane (110) one can see both the regions of extra DED and the regions with the lack of DED (Fig. 9.b). In region 1 the relative lack in DED (– 0.01 e/Å^3) is observed. It is caused by relatively large distances between Be atoms and between Ag and Be atoms in the considered point of this plane. Region 2 in this Figure corresponds to extra DED (+ 0.07 e/Å^3). It is apparently caused by interaction of Be atom located above this region with surrounding Be atoms in the plane (110).

In the plane (110) of Be_2Ti phase in the region 1 DED is equal to – 0.005 e/Å^3. The lack of DED in this region is caused by the redistribution of the electrons that belong to Be atoms above and beneath this plane. The extra DED, which observed in region 2, is equal to + 0.05 e/Å^3. The redistribution of the electrons that belong to Ti atoms surrounding this region (Fig. 9.c) mainly causes this value of DED.

Conclusions

Analysis of total and partial DOS for all studied Laves phases allowed getting information about the nature of chemical bonding in these compounds. Total DOS showed that Al_2Ca is characterized by larger component of metallic bond in comparison with two other compounds. Promoted *d*-electrons of Al participate in covalent bonding which is determined by a superposition of *s*-, *p*- and promoted *d*-states of Al electrons. Promoted *d*-electrons of Al play partly a role of conductive electrons and consequently participate in metallic bonding. Electro-negativities of Al and Ca atoms differ significantly (1.5 and 1.0 accordingly). Thus the ionic component in the bonding is significant. As a result this Laves phase compound is characterized by relatively high structural stability [12].

Considering Be_2Ag, it is possible to conclude that this compound is characterized by smallest component of metallic bonding in comparison with two other compounds. The covalent component of chemical bonding in this phase is somewhat larger. Electro-negativities of Be and Ag atoms are close and therefore the ionic component of chemical bonds in Be_2Ag compound is absent. On the phase diagram it exists in a narrow temperature interval and decomposes to other phases outside this interval.

In Be_2Ti phase we found a degree of metallic bonding that is significantly larger than in Be_2Ag and close to metallic bonding in Al_2Ca. The covalent component in the bonding in Be_2Ti is determined by superposition of *p*-states of Be and *d*-states of Ti. Its value is significantly larger than for Al_2Ca and somewhat less than for Be_2Ag. Electro-negativities of Be and Ti atoms are close, and in this case the ionic component in bonding is negligible. We can expect that structural stability of Be_2Ti is somewhat less in comparison with Al_2Ca.

References

1. Wernic, J. H. *Intermetallic Compounds /* Ed. J. H. Westbook. New York: Wiley, 1967.
2. Sinha, A. K. *Prog. Mater. Sci.,* Vol. 15, part 2, 1972, p. 79.
3. Chaudhary, S., Singh, K. J., Roy, S. B., Chaddah, P. *Physica C. Superconductivity,* Vol. 377, 2002, p. 130.
4. Hishinuma, Y., Kikuchi, A., Iijima, Y., Yoshida, Y., Takeuchi, T., Nishimura, A., Inoue, K. *Fusion Engineering and Design,* Vol. 81, 2006, p. 975.
5. Mohan, Ch. V. *Journal of Alloys and Compounds,* Vol. 238, 1996, p. 86.
6. Strinivas, G., Sankaranayanan, V., Ramapra, S. *Journal of Alloys and Compounds,* Vol. 448, 2008, p. 159.
7. Kumar, K. S., Miracle, D. B. *Intermetallics,* Vol. 2, 1994, p. 257.
8. Toma, D. J., Perepezko, J. H. *Materials Science and Engineering,* Vol. A156, 1992, p. 97.
9. Zhu, J. H., Liu, C. T., Pike, L. M., Liaw, P. K. *Metallurgical and Materials Transactions,* Vol. A30, 1999, p. 1449.
10. Yao, Q., Sun, J., Lin, D., Liu, S., Jiang, B. *Intermetallics,* Vol. 15, 2007, p. 694.
11. Zhang, Ch., Zhang, Z., Wang, S., Li, H., Dong, J., Xing, N., Guo, Y., Li, W. *Journal of Alloys and Compounds,* Vol. 448, p. 53.
12. Zhou, D. W., Liu, J. S., Peng, P., Chen, L., Hu, Y. J. *Materials Letters,* Vol. 62, 2008, p. 206.
13. Kohn, W., Vashishta, P. *General density functional theory, in Theory of the Inhomogeneous Electron gas /* Edited by S. Lundqvist and N. H. March. New York: Plenum, 1983, p. 79.
14. Kohn, W., Becke, A. D., Parr, R. G. *J. Phys. Chem.,* Vol. 100, 1996, p. 12974.
15. Schwarz, K., Blaha, P., Madsen, G. K. H. *Comp. Phys. Comm.,* Vol. 147, 2002, p. 17.
16. Cottenier, S. *Density Functional Theory and the family of (L)APW-methods: a step-by-step introduction.* Belgium: Instituut Voor Kern-en Stralingsfysica, K. U. Leuven, 2002. (http://www,wien2k.at/reg_user/textbooks).
17. Blaha, P., Schwarz, K., Madsen, G., Kvasnicka, D., Luitz, J. *Computer code WIEN2K*. Institute for Materials Chemistry, TU Vienna, 2002.
18. Desclaux, J. P. *Comp. Phys. Commun*., Vol. 1, 1969, p. 216.
19. Koelling, D. D., Harmon, B. N. *J. Phys. C: Slo. St. Phys*., Vol. 10, 1977, p. 3107.
20. Perdew, J. P., Burke, K., Ernzerhof, M. *Physical Review Letters,* Vol. 77, 1996, p. 3865.
21. Blaha, P., Schwartz, K., Madsen, G. K. H., Kvasnicka, D., Luitz, J. *WIEN2k. An augmented plane wave + local orbitals program for calculating crystal properties,* 2001.
22. Smithels, C. J. *Metals Reference Book*. London: Butherworth, 1962.

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CLUSTER EMBEDDING METHOD FOR LARGE ELECTRON SYSTEMS: DIRECT VARIATIONAL APPROACH VERSUS THEORY OF PSEUDOPOTENTIALS

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Problem "cluster in the field of the rest of system" is treated in the frameworks of one-electron approximation with non-orthogonal wave functions. Consideration is general for every task of this type (cluster and the rest of crystal, fragment of a molecule and the remaining part of it, valence and core electrons, etc.). Two alternative approaches are compared:

(A) direct variational approach, when total energy of the whole system (cluster + the rest of system) is expressed in terms of *non-orthogonal* one-electron wave functions and equations for the cluster wave functions are obtained directly from variation of the total energy expression;

(B) approach of the theory of pseudopotentials, when total energy of the system is expressed in terms of *mutually orthogonal* wave functions, equations for the cluster wave functions are obtained under orthogonality constraints and then these equations are transformed to obtain non-orthogonal solutions.

For the both (A) and (B) cases homogeneous equations resulting directly from variational procedure are obtained first. Then these equations are transformed to eigenvalue problem equations. Special case of eigenvalue equations for mutually orthogonal wave functions of the cluster staying to be not orthogonal to the remaining system wave functions is studied. Well-known in the theory of pseudopotentials generalised Phillips–Kleinman (GPK) equations are shown to be particular case of approach (B) eigenvalue equations. Mutually orthogonal wave functions of the cluster are established to be solutions of the equations in the both (A) and (B) cases if additional restrictions on the wave functions are imposed. Unlike theory of pseudopotentials (B), in the case of direct variational approach (A) wave functions of the rest of system are found not to be solutions of the equations for the cluster. It seems to be significant advantage of direct variational approach.

Keywords: *quantum-chemical simulation, embedded molecular cluster (EMC) model, non-orthogonal one-electron wave functions, localised molecular orbitals (LMO), theory of pseudopotentials, generalised Phillips–Kleinman (GPK) equations*

1. Introduction

When we treat infinite or very large electron systems we have to develop approaches giving us opportunity to transform our task to that for small finite part of the whole electron system. Consider main problems we have to deal with when our system has no translation symmetry, so we cannot use it to simplify the task.

Point defect in a crystal is an example of such system. Description of a crystal with a point defect is based on an intuitive assumption that presence of the defect in the crystal alters significantly a finite region of the crystal, including the defect and several spheres of its nearest surrounding. The whole system, i. e. the electrons and nuclei of the crystal with a point defect, may be split on two subsystems: the electrons and nuclei of the defect and its vicinity, and the electrons and nuclei of the remaining crystal. The first subsystem is finite and may be considered as a cluster in the field of the remaining crystal. The second subsystem (remaining crystal) is infinite. Its description is impossible without further approximations and assumptions. While electronic and spatial structures of the cluster are calculated by quantum-chemical methods as precisely as it is possible.

Biological molecule (like DNA or protein) is another example of such system. To solve task for the whole system, we also have to split the system in two parts: small fragment of the molecule and the remaining part of it. To treat large remaining part of the molecule, we have to make further approximations. While small fragment of the molecule may be considered as a cluster in the field of the rest of system.

Trying to obtain equations for the cluster one-electron wave functions, we face with general problem of description of "subsystem in the field of the remaining part of the whole electron system". Task for the cluster and the remaining part of crystal is a particular case of problem of this kind. Other possible cases may be, for example, fragment of a polymer and the remaining part of it, valence and core electrons, etc. All these systems have similar features and may be treated in the frameworks of embedded molecular cluster (EMC) model [1]. Cluster, fragment of a polymer, valence electrons may be treated

as entire quantum-chemical system (cluster). The remaining part (the rest of crystal, the remaining part of polymer, core electrons) of a whole system may be considered to be built of structural elements (SE): SE of perfect crystal, building blocks (fragments) of polymer, and cores of separate atoms. The whole quantum system may be described as a cluster embedded into the rest of the whole system.

At present, several approaches employing strong orthogonality constraints have been developed [1–7] to obtain cluster embedding equations. However, non-orthogonal wave functions of SE may turn out to be more localised than orthogonal ones. (See, for example, work of Anderson [8].) It is significant for practical applications, because expansion of a more localised wave function requires smaller basis set.

The case of non-orthogonal one-electron wave functions with arbitrary degree of localisation has been investigated by Adams and Gilbert [9–13]. Adams and Gilbert have treated self-consistent solutions for the whole system and then searched for a particular form of general equations leading to the separation of the whole system on SE. We have chosen different approach to this problem. Unlike Adams–Gilbert theory, we do not imply that wave functions of the rest of system are self-consistent solutions of the equations for the whole system (cluster + the rest of system). Self-consistent solutions present a particular case for our approach, while equations for the cluster remain mathematically correct if we do not suppose that we know exact self-consistent solutions for the rest of system. It is significant for practical applications because we are pressed to make approximations when we describe the rest of system.

Our task (subsystem in the field of frozen remaining part of the whole system) is classical task of the theory of pseudopotentials. This theory [14–17] is well-developed for molecules for the case of valence electrons in the field of core electrons. In this case the only thing is really significant – valence pseudo wave functions are not orthogonal to the core wave functions. Pseudo wave functions of the valence electrons are not localised wave functions. They are spread over the whole molecule and therefore are considered to be close to delocalised canonical Hartree–Fock molecular orbitals. In our case, in contrast, wave functions of the cluster should be localised in the cluster region. Therefore, they can not be treated like slightly changed canonical Hartree–Fock orbitals, because the latter are delocalised over the whole system (in the case of perfect crystals canonical Hartree–Fock orbitals are Bloch functions). We need adequate equations for the case of localised pseudo wave functions.

In the theory of pseudopotentials approximation of mutually orthogonal frozen cores is used. For core electrons in molecules it is valid quite well and only minor corrections sometimes required. For our case, after dividing the system on SE, the wave functions of SE for the frozen subsystem (the rest of a whole system) overlap with each other in the same way like wave functions of the cluster overlap with those of the rest of system. Indeed, when cluster does not contain defects it is a piece of perfect crystal. In this case the cluster and the rest of crystal are composed of the same SE and therefore all their wave functions overlap in the same manner. Therefore, non-orthogonality of the frozen subsystem SE is significant and should be substantial part of the theory.

In addition, theory of pseudopotentials is well-developed for the case when one-electron states of the varied and the frozen subsystems belong to different parts of energetic spectra with well-defined gap between them. It is true when we treat valence and core electrons, but it is completely wrong in the case of cluster and the rest of crystal, because the cluster and the remaining crystal electron states have the same energy. Situation is the same, too, when we consider fragment of a molecule and the remaining part of it. Therefore, for our case, we should revise theory of pseudopotentials.

To obtain embedding equations for the small part (cluster) of a large system, we should start from the very beginning and derive the most general equations resulting from variational procedure. There are two alternative approaches for the problem “cluster in the field of the rest of system”:

(A) direct variational approach, when total energy of the whole system (cluster + the rest of system) is expressed in terms of *non-orthogonal* one-electron wave functions and equations for the cluster wave functions are obtained directly from variation of the total energy expression;

(B) approach of the theory of pseudopotentials, when total energy of the system is expressed in terms of *mutually orthogonal* wave functions, equations for the cluster wave functions are obtained under orthogonality constraints and then these equations are transformed to obtain non-orthogonal solutions.

Case (A) is already thoroughly studied in our earlier works [18–20]. In the present work we study case (B) and compare two alternative approaches (A) and (B).

2. Cluster Embedding Equations

Start with the review of the most significant results of our earlier works [18, 19] completing our study with new recent results.

2.1. Direct Variation

General scheme of direct variational approach is the following. Total energy of the whole electron system (cluster + the rest of system) is expressed in terms of non-orthogonal one-electron wave functions. Wave functions of the rest of system are considered to be known. Equations for the cluster wave functions are obtained directly from variation of the total energy expression subject to the conditions that wave functions of the rest of system are fixed during variation. Mutual orthogonality restrictions are not imposed during variation. Equations for non-orthogonal cluster wave functions are variational equations.

Considering system of N electrons within one-electron approximation, we may assume that many-electron wave function of the system is represented by a single Slater determinant (it corresponds to calculation of an open shell system by unrestricted Hartree–Fock method). A one-determinant wave function is known to be invariant with respect to arbitrary non-singular linear transformation of the one-electron wave functions (spin-orbitals) included in the determinant [21, 22]. Existence of such transformation allows us to use for description of many-electron system localised one-electron wave functions instead of delocalised ones and to keep many-electron wave function unchanged. Non-singular transformation of one-electron wave functions keeps one-electron density unchanged [21, 22], too. If nature of chemical bonding really permits us to transform delocalised one-electron wave functions to localised ones, we may use ideas of EMC model [1] and divide our N electron system on two subsystems: cluster of finite size and the rest of the system. Then spin-orbitals of the whole electron system $|\Psi_i\rangle$, $i \in$ c + r, may be split on two groups: $|\psi_i\rangle$, $i \in$ c: localised in the cluster region, and $|\varphi_i\rangle$, $i \in$ r: localised in the region of the remaining part of system. Total energy of many-electron system described by non-orthogonal one-electron wave functions may be expressed in the following way:

$$E = \int h(1)\rho(1|2)\big|_{2=1} d1 + \tfrac{1}{2}\int g(1,2)[\rho(1|1)\rho(2|2) - \rho(1|2)\rho(2|1)]d1d2\,, \qquad (1)$$

where $\rho(1|2) = \sum_{i,j \in c+r} \Psi_i(1)\left(S^{-1}\right)_{ij}\Psi_j^*(2)$ is one-electron density;

$h(1) = T(1) + V(1)$ includes electron kinetic energy operator $T(1)$ and operator $V(1)$, which describes interaction of the electrons and nuclei;

$g(1,2) = |\vec{r}_1 - \vec{r}_2|^{-1}$ is operator for interaction between electrons;

and $S_{ij} = \langle \Psi_i | \Psi_j \rangle = \int \Psi_i^*(1)\Psi_j(1)d1$ are one-electron wave functions overlap matrix elements. Electron coordinates includes both spatial and spin variables, the integration is carried out over both of them.

Requiring that the total energy variation δE is zero for arbitrary variations of the cluster wave functions $\delta\psi_l$ and $\delta\psi_k^*$ and transforming variational equations to get in the left side operator acting on the cluster wave functions, we come to the following system of equations [18, 19]:

$$\sum_{k \in c}\sum_{l \in c+r}(1-\rho)F|\Psi_l\rangle\left(S^{-1}\right)_{lk}\langle\psi_k|\psi_i\rangle = 0\,,\ i \in \text{c}, \qquad (2)$$

where ρ is one-electron density operator,

$$\rho = \sum_{i,j \in c+r} |\Psi_i\rangle\left(S^{-1}\right)_{ij}\langle\Psi_j| \qquad (3)$$

F is Fock's operator,

$$F|\psi(1)\rangle = h(1)|\psi(1)\rangle + \int \rho(2|2)g(1,2)|\psi(1)\rangle d2 - \int \rho(1|2)g(1,2)|\psi(2)\rangle d2\,.$$

Defining the following operators:

$$P_c = \sum_{i \in c}\sum_{j \in c+r}|\psi_i\rangle\left(S^{-1}\right)_{ij}\langle\Psi_j|\,, \qquad (4)$$

$$P_r = \sum_{i \in r}\sum_{j \in c+r}|\varphi_i\rangle\left(S^{-1}\right)_{ij}\langle\Psi_j|\,, \qquad (5)$$

we may be write our system of equations in the following way [18, 19]:

$$(1-\rho)FP_c^+\left|\psi_i\right\rangle = 0\ ,\ i\in \mathrm{c}, \tag{6}$$

or, taking into account that $P_c + P_r = \rho = P_c^+ + P_r^+$ it may be rewritten in hermitean form for occupied states:

$$\left(\ \left[1-P_r\right]F\left[1-P_r\right]^+ - P_cFP_c^+\right)\left|\psi_i\right\rangle = 0\ ,\ i\in \mathrm{c}. \tag{7}$$

It is easy to see that every linear combination of the solutions of Eqs. (6) is also solution of these equations. To get linearly independent solutions, in our earlier works [18, 19] we followed ideas of Adams and Gilbert [9–13] and transformed our equations to eigenvalue and eigenvector problem equations:

$$\left(\ \left[1-\rho\right]FP_c^+ + A\right)\left|\psi_i\right\rangle = \lambda_i\left|\psi_i\right\rangle\ ,\ i\in \mathrm{c}. \tag{8}$$

In contrast to Adams and Gilbert we have no demanded for operator A to be hermitean.
To get Eqs. (6) as the consequence of Eqs. (8), the following restriction must be imposed on A [18, 19]:

$$\rho A\left|\psi_i\right\rangle = A\left|\psi_i\right\rangle\ ,\ i\in \mathrm{c}. \tag{9}$$

Under this restriction Eqs. (8) lead to Eqs. (6) and additional condition [18, 19]:

$$A\left|\psi_i\right\rangle = \lambda_i\left|\psi_i\right\rangle\ , i\in \mathrm{c}. \tag{10}$$

If operator A is properly chosen spectral problem (8) has non-degenerate linearly independent solutions.

For practical applications it is important to consider the case when cluster one-electron wave functions are mutually orthogonal but stay to be not orthogonal to the remaining system one-electron wave functions. To get mutually orthogonal solutions, we must obtain eigenvalue and eigenvector problem for hermitean operator with non-degenerate spectrum. In our earlier works [18, 19] we proposed the following equations:

$$\left(\ \left[1-P_r\right]F\left[1-P_r\right]^+ + P_cGP_c^+\right)\left|\psi_i\right\rangle = E_i\left|\psi_i\right\rangle\ ,\ i\in \mathrm{c}, \tag{11}$$

where G is hermitean operator.

If operator G is properly chosen spectral task (11) has non-degenerate mutually orthogonal solutions. If we choose $G = 0$ we get the following equations:

$$\left(1-P_r\right)F\left(1-P_r\right)^+\left|\psi_i\right\rangle = E_i\left|\psi_i\right\rangle\ ,\ i\in \mathrm{c}. \tag{12}$$

Equations (12) coincide with those obtained by H. Stoll with co-workers [23, 24]. They present not general, but very important case of equations for mutually orthogonal cluster wave functions. Using cluster embedding equations (12) we have developed modified cluster embedding scheme and have demonstrated that consistent implementation of this scheme may radically reduce boundary effects in EMC model [19, 25].

2.2. Properties of "Pseudoprojectors"

In our earlier works [18, 19] we have shown that operators P_c and P_r

a) are idempotent

$$\left(P_c\right)^2 = P_c\ , \qquad \left(P_r\right)^2 = P_r\ ;$$

b) are invariant with respect to linear transformation of the cluster states;
c) are invariant with respect to linear transformation of the remaining system states, too;
d) may be decomposed on projectors and rotation operators.

Consider the latter property with more details. Because the cluster and the remaining system wave functions are linearly independent, without loss of generality wave functions of the cluster may be expressed as follows:

$$\left|\psi_i\right\rangle = \left|\phi_i\right\rangle + \sum_{j\in r}\left|\varphi_j\right\rangle\ a_{ji}\ ,\ i\in \mathrm{c}, \tag{13}$$

where

$|\varphi_j\rangle$, $j \in$ r, are wave functions of the rest of system, they are not mutually orthogonal, $\langle\varphi_i|\varphi_j\rangle = (S_r)_{ij}$;

$|\phi_i\rangle$, $i \in$ c, are orthogonal to the rest of system components of the cluster wave functions, $\langle\phi_i|\varphi_j\rangle = 0$, they are linearly independent but in general case are not mutually orthogonal, $\langle\phi_i|\phi_j\rangle = B_{ij}$;

coefficients a_{ji} describe overlaps between the cluster and the rest of system wave functions.

Substituting expansion (13) in the definitions of operators P_c and P_r (see formulas (4) and (5) and use final results of Appendix) we get [18, 19]:

$$P_c = W_c + R_c, \tag{14}$$

$$P_r = \Omega_r - R_c. \tag{15}$$

First terms in the expressions (14) and (15) are projection operators. Projector W_c is defined as follows:

$$W_c = \sum_{i,j\in c} |\phi_i\rangle (B^{-1})_{ij} \langle\phi_j|; \tag{16}$$

projector Ω_r is projector on the remaining system wave functions space:

$$\Omega_r = \sum_{i,j\in r} |\varphi_i\rangle (S_r^{-1})_{ij} \langle\varphi_j|, \tag{17}$$

where S_r is matrix of overlaps between the wave functions of the remaining system.

Rotation operator R_c is defined as follows:

$$R_c = \sum_{i\in r}\sum_{j\in c} |\varphi_i\rangle (A_c B^{-1})_{ij} \langle\phi_j|, \tag{18}$$

where matrix A_c is matrix of coefficients a_{ji} in expansion (13) for the cluster wave functions.

Taking into account that $P_r + P_c = \rho$ and substituting (14) and (15) it is easy to see that sum of projectors W_c and Ω_r gives one-electron density operator (3) for the whole system: $\Omega_r + W_c = \rho$.

2.3. Theory of Pseudopotentials

In this section we obtain embedding equations for the cluster wave functions using ideas of the theory of pseudopotentials (case B). Usual suppositions accepted in the theory of pseudopotentials are the following (see, for example, the monograph of Szasz [14]). Wave function of a many-electron system is taken in a form of a Slater determinant constructed from mutually orthogonal one-electron wave functions. Then the electron system is divided on two subsystems. Wave functions of the first subsystem, $|\varphi_i\rangle$, $i \in$ r, are assumed to be known and fixed. Equations for the wave functions of the second subsystem, $|\phi_i\rangle$, $i \in$ c, are obtained from the requirement of a minimum of the total energy of the whole electron system under the orthogonality constraints on the one-electron wave functions. Total energy of the system is varied subject to the condition that wave functions of the first subsystem are frozen and are not varied. For our case the second subsystem (varied subsystem) is cluster and the first subsystem (frozen subsystem) is the rest of the whole system. Variation procedure leads to non-canonical Hartree–Fock equations for the cluster wave functions:

$$F|\phi_i\rangle = \sum_{j\in c} |\phi_j\rangle E_{ji} + \sum_{j\in r} |\varphi_j\rangle E_{ji}, \quad i \in \text{c}. \tag{19}$$

It is usually considered that off-diagonal Lagrange multipliers intermixing the varied subsystem (cluster) wave functions with each other are equal to zero:

$$F|\phi_i\rangle = E_i|\phi_i\rangle + \sum_{j\in r} |\varphi_j\rangle E_{ji}, \quad i \in \text{c}. \tag{20}$$

In this way, substituting expression for Lagrange multipliers $E_{ji} = \langle \varphi_j | F | \phi_i \rangle$, Eqs. (20) are rewritten using projection operators:

$$F|\phi_i\rangle = E_i|\phi_i\rangle + \sum_{j\in r} |\varphi_j\rangle\langle\varphi_j|F|\phi_i\rangle, \ i\in \mathrm{c}. \tag{21}$$

Then wave functions of varied subsystem (cluster) $|\phi_i\rangle$, $i\in$c, are replaced by $|\psi_i\rangle$, $i\in$c, called pseudo functions. "True" wave functions $|\phi_i\rangle$ are orthogonal to the wave functions of the frozen subsystem (the rest of the whole system) $|\varphi_i\rangle$, $i\in$r, while pseudo functions $|\psi_i\rangle$ already are not orthogonal to the wave functions of the frozen subsystem. Pseudo functions are supposed to be connected with "true" wave functions in the following way:

$|\psi_i\rangle = |\phi_i\rangle + \sum_{j\in r} |\varphi_j\rangle a_{ji}$ (expansion of form (13)),

$$|\phi_i\rangle = (1-\Omega_r)\,|\psi_i\rangle, \tag{22}$$

where $\Omega_r = \sum_{j\in r} |\varphi_j\rangle\langle\varphi_j|$ is the projector on the frozen subsystem (the rest of the whole system) wave function space.

Substituting (22) in (21) we obtain generalised Phillips–Kleinman (GPK) equations [14–17]:

$$(1-\Omega_r)F(1-\Omega_r)\,|\psi_i\rangle = E_i(1-\Omega_r)\,|\psi_i\rangle, \ i\in \mathrm{c}. \tag{23}$$

Transforming in the same manner equations (19) resulting from variational procedure in general case, we finally get [18]:

$$(1-\rho)F(1-\Omega_r)\,|\psi_i\rangle = 0, \ i\in \mathrm{c}. \tag{24}$$

Deriving Eqs. (24) we have taken into account that relationships (22) are a particular case of linear transformation of the wave functions and, therefore, one-electron density operator ρ may be written in the following way:

$$\rho = \sum_{j\in c} |\phi_j\rangle\langle\phi_j| + \sum_{j\in r} |\varphi_j\rangle\langle\varphi_j| = \sum_{i,j\in c+r} |\Psi_i\rangle (S^{-1})_{ij} \langle\Psi_j|, \text{ where } |\Psi_i\rangle = \begin{cases} |\varphi_i\rangle, & i\in \mathrm{r} \\ |\psi_i\rangle, & i\in \mathrm{c} \end{cases}, \ S_{ij} = \langle\Psi_i|\Psi_j\rangle.$$

Therefore, the most general equations of the theory of pseudopotentials are our equations (24), while GPK equations (23) present a particular case.

Note that every linear combination of the solutions of Eqs. (24) is also solution of these equations, analogously to Eqs. (6) obtained in the frameworks of direct variational approach. Using arguments similar to those listed in Sect. 2.1, we may propose the following eigenvalue and eigenvector equations [18]:

$$\left([1-\rho]F[1-\Omega_r] + A \right) |\psi_i\rangle = \lambda_i |\psi_i\rangle, \ i\in \mathrm{c}. \tag{25}$$

Analogously to direct variational approach, if we want solutions of Eqs. (25) to be solutions of Eqs. (24), restriction (9) must be imposed on operator A, and under this restriction Eqs. (25) lead not only to Eqs. (24) but also to additional condition (10). Analogously to Eqs. (8) solutions of Eqs. (25) should be interpreted as those of Eqs. (24) under additional condition (10). Eqs. (25) may be considered as the most general eigenvalue and eigenvector equations of pseudopotential theory. Condition (9) restricts freedom of choice of the pseudopotential.

Establish now for what operator A Eqs. (25) convert to GPK equations (23). For this purpose it is necessary to get rid of an explicit energetic dependence of operators in Eqs. (23) expressing E_i and substituting this expression into the equations. In this way, using previously defined operator P_r (5) and formulas of Appendix we obtain equations without explicit energetic dependence of operators [18]:

$$(1-P_r)F(1-\Omega_r)\,|\psi_i\rangle = E_i|\psi_i\rangle, \ i\in \mathrm{c}. \tag{26}$$

Eqs. (26) are special case of eigenvalue and eigenvector equations (25) with $A = P_c F(1-\Omega_r)$. It is easy to see that for this A restriction (9) is valid.

We should note that the wave functions of the frozen subsystem $|\varphi_i\rangle$, $i \in$ r, are solutions of the both Eqs. (23) and (26), but for Eqs. (26) the energy E_i is equal to zero while in original GPK equations (23) the energy E_i is arbitrary. This arbitrariness of the energy is the reason of arbitrary admixture of the wave functions of the frozen subsystem in the solutions of GPK equations for the cluster. Investigate whether Eqs. (26) keep this feature for both occupied and vacant states or not. Transformation procedure we have used to get Eqs. (26) is valid for occupied states only. Therefore, vacant states require special consideration.

3. Vacant States

Further applications of EMC model require us to go beyond one-electron approximation and to use one of existing methods including many-electron correlation effects into consideration (to calculate optical transition energies or magnetic resonance effects, for example). To apply any of these methods, we need initial eigenvalue equations giving the same structure and the same degree of localisation for the both vacant and occupied cluster states. Equations for the cluster wave functions may give solutions of different structure for occupied states and for vacant ones. In this section we study this problem with more details.

We may define vacant solutions as extra solutions staying linearly independent with the cluster and the rest of the system occupied states. According to this definition $\rho|\psi_i\rangle \neq |\psi_i\rangle$, $i \in$ v, but not necessarily $\rho|\psi_i\rangle = 0$. It means that like occupied cluster states vacant states without loss of generality may be described by formula (13).

3.1. GPK Equations

Start with Eqs. (26) and establish structure of their solutions for the both occupied and vacant states. To get these equations, we transformed GPK equations. Ascertain that original GPK equations (23) are consequence of our equations (26).

Taking into account that $\Omega_r P_r = P_r$ (see definition (5) of P_r) we see that

$$(1-\Omega_r)(1-P_r) = 1-\Omega_r .$$

Therefore, acting on the left and the right sides of Eqs. (26) by $(1-\Omega_r)$ we have:

$$(1-\Omega_r)(1-P_r)F(1-\Omega_r)|\psi_i\rangle = (1-\Omega_r)E_i|\psi_i\rangle ,$$

$$(1-\Omega_r)F(1-\Omega_r)|\psi_i\rangle = E_i(1-\Omega_r)|\psi_i\rangle .$$

We see that GPK equations (23) really are consequence of our equations (26). Establish now have solutions of Eqs. (26) arbitrary admixture of frozen subsystem wave functions or not. Using expression (15) for P_r we may rewrite Eqs. (26) in the following way:

$$\left[(1-\Omega_r)+R_c\right]F(1-\Omega_r)|\psi_i\rangle = E_i|\psi_i\rangle .$$

Acting on the both left and right sides of these equations by Ω_r and taking into account that $\Omega_r R_c = R_c$ (see definition (18) of R_c) we get:

$$R_c F(1-\Omega_r)|\psi_i\rangle = E_i\Omega_r|\psi_i\rangle . \tag{27}$$

Rearranging terms in GPK equations we have:

$$F(1-\Omega_r)|\psi_i\rangle = E_i(1-\Omega_r)|\psi_i\rangle + \Omega_r F(1-\Omega_r)|\psi_i\rangle . \tag{28}$$

Taking into account that GPK equations are consequence of our equations (26) and substituting expression (28) in the left part of (27) we get:

$$R_c E_i(1-\Omega_r)|\psi_i\rangle + R_c\Omega_r F(1-\Omega_r)|\psi_i\rangle = E_i\Omega_r|\psi_i\rangle .$$

Substituting expansion (13) for $|\psi_i\rangle$ and taking into account that $R_c\Omega_r = 0$ (see definition (18) of R_c) we come to:

$$E_i R_c|\phi_i\rangle = E_i \sum_{j\in r} |\varphi_j\rangle\ a_{ji}\ . \tag{29}$$

So, on one hand, if solutions of Eqs. (26) are expressed by expansion (13), expansion coefficients and wave functions satisfy Eqs. (29). On the other hand, if we substitute expansion (13) for $|\psi_i\rangle$ in GPK equations (23) (we have shown that GPK equations are consequence of our equations), we get Huzinaga equations [2, 3] for $|\phi_i\rangle$:

$$(1-\Omega_r)F|\phi_i\rangle = E_i|\phi_i\rangle, \tag{30}$$

what means that wave functions $|\phi_i\rangle$ in expansion (13) are mutually orthogonal for all (occupied and vacant) cluster states.

Solutions of Eqs. (26) will contain arbitrary admixture of frozen subsystem wave functions if equations (29) reduce to an identity. According to definition of R_c

$$R_c|\phi_i\rangle = \sum_{j\in r}\sum_{k\in c} |\varphi_j\rangle\left(A_c B^{-1}\right)_{jk}\langle\phi_k|\phi_i\rangle,\ \ i\in \mathrm{c + v}.$$

Therefore, for occupied cluster states

$$R_c|\phi_i\rangle = \sum_{j\in r}\sum_{k\in c} |\varphi_j\rangle\left(A_c B^{-1}\right)_{jk} B_{ki} = \sum_{j\in r}|\varphi_j\rangle a_{ji}\ ,\ \ i\in \mathrm{c},$$

and (29) really converts to identity. But for vacant ones due to mutual orthogonality of $|\phi_i\rangle$, $i\in$ c + v, $\langle\phi_k|\phi_i\rangle = 0$ when $k\in$ c and $i\in$ v. It means that for vacant states $R_c|\phi_i\rangle = 0$ and we have zero in the left side of formula (29). Therefore, the right side should be zero, too. Formula (29) is valid for the both occupied and vacant cluster states. Therefore, all $a_{ji} = 0$ for vacant solutions of Eqs. (26). It means that vacant states are orthogonal to the both varied (cluster) and frozen (the rest of the whole system) subsystems occupied states:

$$(1-\rho)\,|\psi_i\rangle = |\psi_i\rangle,\ \ i\in \mathrm{v}. \tag{31}$$

Taking it into account and acting on the both left and right parts of Eqs. (26) by $(1-\rho)$ we get the following equations for vacant states:

$$(1-\rho)F|\psi_i\rangle = E_i|\psi_i\rangle,\ \ i\in \mathrm{v}. \tag{32}$$

It means that vacant solutions of Eqs. (26) are canonical Hartree–Fock orbitals. They are orthogonal to the occupied states both of the cluster and of the rest of system. Operator $(1-\rho)$ in the left side ensures this orthogonality.

Summing up, we conclude that solutions of Eqs. (26) have arbitrary admixture of frozen subsystem wave functions for occupied states only. Therefore, Eqs. (26) are not equivalent to GPK equations for vacant states of varied subsystem (cluster). To reach complete equivalence, we should modify our equations.

By analogy with rotation operator R_c for occupied cluster states define rotation operator R_v for vacant states:

$$R_v = \sum_{j\in r}\sum_{k\in v} |\varphi_j\rangle\left(A_v D^{-1}\right)_{jk}\langle\phi_k|, \tag{33}$$

where $|\varphi_j\rangle$, $j\in$r, $|\phi_k\rangle$, $k\in$v, are wave functions and A_v is matrix of coefficients a_{ji} in expansion of form (13) for vacant states; $|\phi_k\rangle$, $k\in$v, belong to orthogonal to the both cluster and the rest of system occupied wave functions space, $\langle\phi_i|\phi_k\rangle = 0$, $\langle\varphi_j|\phi_k\rangle = 0$, $i\in$c, $j\in$r, $k\in$v; $D_{ij} = \langle\phi_i|\phi_j\rangle$, $i,\ j\in$v.

It is easy to see that operators R_c and R_v have the following properties:

$$R_c|\varphi_i\rangle = 0\,,\ i\in\mathrm{r}, \qquad R_c|\phi_i\rangle = 0\,,\ i\in\mathrm{v}, \qquad R_c|\phi_i\rangle = \sum_{j\in r}|\varphi_j\rangle a_{ji}\,,\ i\in\mathrm{c};$$

$$R_v|\varphi_i\rangle = 0\,,\ i\in\mathrm{r}, \qquad R_v|\phi_i\rangle = 0\,,\ i\in\mathrm{c}, \qquad R_v|\phi_i\rangle = \sum_{j\in r}|\varphi_j\rangle a_{ji}\,,\ i\in\mathrm{v};$$

$$\text{while } (R_c + R_v)\,|\phi_i\rangle = \sum_{j\in r}|\varphi_j\rangle\ a_{ji}\,,\ \ i\in\mathrm{c}+\mathrm{v}. \tag{34}$$

Therefore, if we want to get the same structure (arbitrary coefficients a_{ji}) for the both occupied and vacant states, instead of operator R_c we need sum of operators R_c and R_v. Modify Eqs. (26) replacing operator $(1-P_r) = (1-\Omega_r) + R_c$ by operator $(1-\Omega_r) + R_c + R_v$:

$$\left[\ (1-\Omega_r) + R_c + R_v\right] F(1-\Omega_r)\ |\psi_i\rangle = E_i|\psi_i\rangle\,. \tag{35}$$

After this modification we also obtain original GPK equations (23) as a consequence our equations (35). It is easy to see it acting on the both the left and the right sides of Eqs. (35) by $(1-\Omega_r)$ and taking into account that $\Omega_r R_v = R_v$ (similarly to $\Omega_r R_c = R_c$).

Presence of rotation operators R_c and R_v in Eqs. (35) causes explicit dependence of the both occupied and vacant states on coefficients a_{ji} in expansion (13). These coefficients describe admixture of frozen subsystem wave functions in the wave functions of varied subsystem. Like in original GPK equations this admixture is arbitrary, but due to explicit dependence we have possibility to set admixture coefficients and to fix them.

We may conclude that modified equations (35) are equivalent to GPK equations for the both vacant and occupied states of the varied subsystem (cluster). Our initial equations (26) are equivalent to GPK equations for occupied states only. Vacant solutions of Eqs. (26) satisfy Eqs. (32). Therefore, transformed form of GPK equations is Eqs. (35).

For the frozen subsystem (the rest of the whole system) equivalence of the equations is not complete. Wave functions of the frozen subsystem are solutions of the transformed and original GPK equations, but with zero energy for Eqs. (35) and arbitrary energy for GPK equations (23).

Eqs. (35) are particular case of eigenvalue and eigenvector equations (25) with $A = (P_c + R_v)F(1-\Omega_r)$. It is easy to see that for this A restriction (9) is valid. So, GPK equations have transformed form (35) and may be considered as special case of eigenvalue and eigenvector equations (25) with particular choice of operator A.

3.2. Direct Variational Equations

In our earlier work [20] we have studied vacant solutions of eigenvalue equations (12) obtained in the frameworks of direct variational approach. We have established that situation is the same as in the case of GPK equations. Vacant solutions of Eqs. (12) satisfy Eqs. (32) and therefore are canonical Hartree–Fock orbitals. To get vacant and occupied states of the same structure, we have to modify our initial equations (12) replacing operator $(1-P_r) = (1-\Omega_r) + R_c$ by operator $(1-\Omega_r) + R_c + R_v$:

$$\left(\ [1-\Omega_r] + R_c + R_v\right) F\left(\ [1-\Omega_r] + R_c^+ + R_v^+\right)|\psi_i\rangle = E_i|\psi_i\rangle\,,\ \ i\in\mathrm{c}+\mathrm{v}. \tag{36}$$

To keep occupied states the same for the both original and modified equations, we have to impose orthogonality restrictions between non-orthogonal to the frozen subsystem components of the occupied cluster states and those of vacant ones [20]:

$$A_v^+ S_r A_c = 0 \qquad \text{or its hermitean conjugate} \qquad A_c^+ S_r A_v = 0\,. \tag{37}$$

Under these restrictions initial equations (12) and modified equations (36) give the same wave functions for occupied cluster states.

4. Comparison of the Approaches

4.1. Varied Subsystem (Cluster)

Study now what kind of solutions pseudopotential theory equations and direct variational equations give for varied subsystem (cluster). Compare solutions of the Eqs. (35) and Eqs. (36) and establish may they be common or not.

If we consider that cluster wave functions $|\psi_i\rangle$, $i \in$ c + v, are described by expansion (13), then, taking into account (37), we get:

$$(1-\Omega_r)\,|\psi_i\rangle = |\phi_i\rangle,\ i \in \text{c+v},$$

$$\left(R_c^+ + R_v^+\right)|\psi_i\rangle = \begin{cases} \sum\limits_{j\in c} |\phi_j\rangle \left(B^{-1}A_c^+ S_r A_c\right)_{ji}, & i \in \text{c} \\ \sum\limits_{j\in v} |\phi_j\rangle \left(D^{-1}A_v^+ S_r A_v\right)_{ji}, & j \in \text{v} \end{cases}. \tag{38}$$

It means that operator $(1-\Omega_r) + R_c^+ + R_c^+$ does not mix occupied and vacant states with each other.

Substituting expansion (13) for the cluster wave functions $|\psi_i\rangle$ on the left side of Eqs. (35) and Eqs. (36), we see that Eqs. (35) give

$$\left([1-\Omega_r] + R_c + R_v \right) F|\phi_i\rangle = E_i|\psi_i\rangle,\ i \in \text{c} + \text{v}, \tag{39}$$

while, taking into account formula (38), for Eqs. (36) we have

$$\left([1-\Omega_r] + R_c + R_v \right) F \sum_{j\in c+v} |\phi_j\rangle\, U_{ji} = E_i|\psi_i\rangle,\ i \in \text{c} + \text{v}, \tag{40}$$

where matrix U is expressed as follows

$$U = \begin{pmatrix} I_c + B^{-1}A_c^+ S_r A_c & 0 \\ 0 & I_v + D^{-1}A_v^+ S_r A_v \end{pmatrix}, \tag{41}$$

I_c and I_v are unit matrices.

Comparing (39) and (40) we see that Eqs. (35) and Eqs. (36) have the same solutions if matrix U is diagonal matrix.

In our earlier work [18] we have studied solutions of Eqs. (12) and Eqs. (26). We have shown that solutions of Eqs. (12) and Eqs. (26) are the same wave functions if we impose additional restrictions related to the cluster and the rest of system wave functions overlaps:

$$\left(A_c^+ S_r A_c\right)_{ij} = 0,\ i \neq j. \tag{42}$$

Being eigenvectors of hermitean operator, solutions of Eqs. (36) are mutually orthogonal. Taking it into account it is possible to show that matrix U has diagonal form if in addition to conditions (37) we impose conditions (42) and the same conditions for vacant states:

$$\left(A_v^+ S_r A_v\right)_{ij} = 0,\ i \neq j. \tag{43}$$

Under these restrictions off-diagonal elements of matrix U are equal to zero while diagonal ones have the following form:

$$U_{ii} = \left(1 + \frac{r_i}{m_i}\right),\ i \in \text{c} + \text{v}, \tag{44}$$

where $m_i = \langle\phi_i|\phi_i\rangle$ and $r_i = \left(A^+ S_r A\right)_{ii}$.

If matrix U has diagonal form (44), the same wave functions $|\psi_i\rangle$, $i \in \mathrm{c} + \mathrm{v}$, are solutions of the both equations (35) and (36). While eigenvalues differ. We have E_i for Eqs. (35) and $\widetilde{E}_i$ for Eqs. (36). It is easy to see that eigenvalues are related with each other as follows:

$$\widetilde{E}_i = E_i\left(1 + \frac{r_i}{m_i}\right), \quad i \in \mathrm{c} + \mathrm{v}.$$

Conditions (37), (42) and (43) impose mutual orthogonality restrictions on non-orthogonal to the rest of system components of the cluster wave functions. It is easy to prove that these conditions ensure mutual orthogonality of solutions for Eqs. (35). It is additional restriction. In contrast with solutions of Eqs. (36), solutions of Eqs. (35) are not mutually orthogonal in general case.

4.2. Frozen Subsystem (the Rest of the Whole System)

Wave functions of the frozen subsystem (the rest of the whole system) are solutions of the equations obtained in the framework of the theory of pseudopotentials because $(1 - \Omega_r)|\varphi_i\rangle = 0$, $i \in r$. In our previous work [18] we have shown that wave functions of the frozen subsystem are not solutions of eigenvalue equations (12). Investigate, whether it is true or not for modified equations (36).

By analogy with projector W_c and pseudoprojector P_c for occupied states define projector W_v and pseudoprojector P_v for vacant states:

$$W_v = \sum_{i,j \in v} |\phi_i\rangle (D^{-1})_{ij} \langle \phi_j|, \tag{45}$$

$$P_v = W_v + R_v. \tag{46}$$

Then, according to formulas (17), (14), (46), (16) and (45), for the frozen subsystem wave functions $|\varphi_i\rangle$, $i \in r$, we have the following result:

$$\left([1 - \Omega_r] + R_c^+ + R_v^+ \right)|\varphi_i\rangle = \left(R_c^+ + R_v^+\right)|\varphi_i\rangle = \left(P_c^+ - W_c + P_v^+ - W_v\right)|\varphi_i\rangle = P_c^+|\varphi_i\rangle + P_v^+|\varphi_i\rangle. \tag{47}$$

Therefore, for our purpose it is enough to consider the result of action of pseudoprojectors P_c^+ and P_v^+ on the frozen subsystem wave functions.

Taking into account P_c definition (4) and expansion (13), it is possible to see that

$$P_c^+|\varphi_i\rangle = \sum_{k \in c+r} \sum_{j \in c} |\Psi_k\rangle (S^{-1})_{kj} \langle \psi_j|\varphi_i\rangle = \sum_{k \in c+r} \sum_{j,l \in c} |\Psi_k\rangle (S^{-1})_{kl} (S_c S_c^{-1})_{lj} (A_c^+ S_r)_{ji} =$$
$$= \sum_{k \in c+r} \sum_{j,l \in c} |\Psi_k\rangle (S^{-1})_{kl} \langle \psi_l|\psi_j\rangle (S_c^{-1} A_c^+ S_r)_{ji} = P_c^+ \sum_{j \in c} |\psi_j\rangle (S_c^{-1} A_c^+ S_r)_{ji}.$$

So, on one hand, we have just shown that

$$P_c^+|\varphi_i\rangle = P_c^+ \sum_{j \in c} |\psi_j\rangle (S_c^{-1} A_c^+ S_r)_{ji}, \quad i \in \mathrm{r}, \tag{48}$$

and in the similar manner we may show that

$$P_v^+|\varphi_i\rangle = P_v^+ \sum_{j \in v} |\psi_j\rangle (S_v^{-1} A_v^+ S_r)_{ji}, \quad i \in \mathrm{r}. \tag{49}$$

On the other hand, taking into account formulas (14), (46), (17), (16), (45), expansion (13) and condition (37), we get

$$\left([1 - \Omega_r] + R_c^+ + R_v^+ \right)|\psi_i\rangle = \left([1 - \Omega_r] + P_c^+ - W_c + P_v^+ - W_v \right)|\psi_i\rangle = \begin{cases} P_c^+|\psi_i\rangle, & i \in \mathrm{c} \\ P_v^+|\psi_i\rangle, & i \in \mathrm{v} \end{cases}. \tag{50}$$

Summing up results given by formulas (47)–(50), we see that

$$\left(\left[1-\Omega_r\right]+R_c+R_v\right) F\left(\left[1-\Omega_r\right]+R_c^+ +R_v^+\right)\left|\varphi_i\right\rangle =$$

$$=\left(\left[1-\Omega_r\right]+R_c+R_v\right) F\left(\left[1-\Omega_r\right]+R_c^+ +R_v^+\right)\left(\sum_{j\in c}\left|\psi_j\right\rangle\left(S_c^{-1}A_c^+S_r\right)_{ji}+\sum_{j\in v}\left|\psi_j\right\rangle\left(S_v^{-1}A_v^+S_r\right)_{ji}\right).$$

Assuming that $\left|\psi_i\right\rangle$, $i\in$c + v, are solutions of the equations (36), we come to

$$\left(\left[1-\Omega_r\right]+R_c+R_v\right)F\left(\left[1-\Omega_r\right]+R_c^+ +R_v^+\right)\left|\varphi_i\right\rangle =$$

$$=\sum_{j\in c}E_j\left|\psi_j\right\rangle\left(S_c^{-1}A_c^+S_r\right)_{ji}+\sum_{j\in v}E_j\left|\psi_j\right\rangle\left(S_v^{-1}A_v^+S_r\right)_{ji} \quad , \quad i\in \text{r}.$$

Substituting in the last expression expansion (13) for $\left|\psi_i\right\rangle$, $i\in$c + v, we get

$$\left(\left[1-\Omega_r\right]+R_c+R_v\right)F\left(\left[1-\Omega_r\right]+R_c^+ +R_v^+\right)\left|\varphi_i\right\rangle =$$

$$=\sum_{j\in c}E_j\left|\phi_j\right\rangle\left(S_c^{-1}A_c^+S_r\right)_{ji}+\sum_{j\in v}E_j\left|\phi_j\right\rangle\left(S_v^{-1}A_v^+S_r\right)_{ji}+ \quad , \quad i\in \text{r}. \tag{51}$$

$$+\sum_{j\in c}\sum_{k\in r}E_j\left|\varphi_k\right\rangle a_{kj}\left(S_c^{-1}A_c^+S_r\right)_{ji}+\sum_{j\in v}\sum_{k\in r}E_j\left|\varphi_k\right\rangle a_{kj}\left(S_v^{-1}A_v^+S_r\right)_{ji}$$

From (51) we see, that $\left|\varphi_i\right\rangle$, $i\in$r, may be solutions of Eqs. (36) if

$$\sum_{j\in c}E_j\left|\phi_j\right\rangle\left(S_c^{-1}A_c^+S_r\right)_{ji}=0 \text{ and } \sum_{j\in v}E_j\left|\phi_j\right\rangle\left(S_v^{-1}A_v^+S_r\right)_{ji}=0\,. \tag{52}$$

Conditions (52) are necessary conditions for the wave functions of the rest of system (frozen subsystem) to be solutions of equations for the cluster (varied subsystem).

Wave functions $\left|\phi_j\right\rangle$, $j\in$c + v, in the expression (13) are linearly independent. Therefore, to satisfy conditions (52), we have to demand that

a) wave functions of the cluster are orthogonal to those of the rest of system, $\left(A_c\right)_{ji}=0$ and $\left(A_v\right)_{ji}=0$;

or

b) all the eigenvalues E_j are zeros, what is rather doubtful.

We see that wave functions of the rest of system are solutions of the equations for the cluster only if additional conditions are imposed. These conditions are demanding for the wave functions of the cluster to be orthogonal to those of the rest of system. In general case wave functions of the rest of system are not orthogonal to those of the cluster. Non-orthogonality is main assumption of our theory. It means that in general case (when we keep non-orthogonality) conditions (52) are never satisfied. Therefore, on contrast with the theory of pseudopotentials, in the case of Eqs. (36) wave functions of frozen subsystem (the rest of the whole system) are not solutions of the equations for varied subsystem (cluster). It may be significant advantage of direct variational approach.

Summary and Conclusions

We have compared two different approaches to the general problem "cluster in the field of the remaining part of system":

(A) direct variational approach, when total energy of the whole system (cluster + the rest of system) is expressed in terms of *non-orthogonal* one-electron wave functions and equations for the cluster wave functions are obtained directly from variation of the total energy expression;

(B) approach of the theory of pseudopotentials, when total energy of the system is expressed in terms of *mutually orthogonal* wave functions, equations for the cluster wave functions are obtained under orthogonality constraints and then these equations are transformed to obtain non-orthogonal solutions.

For the both (A) and (B) cases we have obtained general (homogeneous) equations (describing linear space of the cluster wave functions) and have transformed them to eigenvalue and eigenvector problem equations (selecting a basis for this space).

We have shown that well-known in the theory of pseudopotentials generalised Phillips–Kleinman (GPK) equations may be transformed to eigenvalue and eigenvector equations. Eigenvalue form of GPK equations – Eqs. (35) is special case of approach (B) eigenvalue and eigenvector equations – Eqs. (25).

We have established that GPK equations and eigenvalue equations of direct variational approach may give the same solutions for the varied subsystem (cluster) under additional restrictions on the wave functions. The same wave functions are solutions of the both equations if we demand mutual orthogonality of the wave functions components describing overlaps of varied wave functions with the frozen ones.

We have found that in the case of approach (A) wave functions of the frozen subsystem (the rest of the whole system) are not solutions of our equations for the varied subsystem (cluster). Pseudopotential theory equations have no this feature. Possibility to formulate task in such a way that wave functions of the frozen subsystem do not appear when we solve equations for the varied subsystem seems to be significant advantage of direct variational approach.

Applicability of our embedding scheme for treatment of electron excited states has been studied. To consider electron transitions, both occupied and vacant states should be localised in the cluster region and should overlap with the rest of system in the same manner. We have established that our initial embedding equations give different localisation degree for occupied and vacant states. For the both approaches (A) and (B) occupied states have localised wave functions while vacant ones are described by delocalised canonical orbitals. We have demonstrated that it is possible to overcome this limitation modifying our initial equations. Treatment of electron excited states and consideration of electron transitions become possible. EMC model with non-orthogonal wave functions becomes applicable for theoretical study of various processes.

Because we have no used specific features of particular systems, our consideration is general for every task "subsystem in the field of the frozen remaining part of the whole electron system". Results of our present work may be used for treatment of all possible tasks of this kind: cluster and the rest of crystal, fragment of a molecule and the remaining part of it, valence and core electrons, fragment of nanosystem and the rest of it, etc.

References

1. Kantorovich, L. N. An embedded-molecular-cluster method for calculating the electronic structure of point defects in non-metallic crystals. I. General theory, *J Phys C: Solid State Phys.,* Vol. 21, 1988, pp. 5041–5056; An embedded-molecular-cluster method for calculating the electronic structure of point defects in non-metallic crystals. II. Structural elements in a form of molecules, *J Phys C: Solid State Phys.,* Vol. 21, 1988, pp. 5057–5073.
2. Huzinaga, S. and Cantu, A. A. Theory of separability of many-electron systems, *J Chem Phys.,* Vol. 55, 1971, pp. 5543–5549.
3. Huzinaga, S., Mc Williams, D. and Cantu, A. A. Projection operators in Hartree–Fock theory, *Adv Quantum Chem.,* Vol. 7, 1973, pp. 187–220.
4. Barandiaran, Z. and Seijo, L. The ab initio model potential representation of the crystalline environment. Theoretical study of the local distortion on NaCl:Cu^+, *J Chem Phys.,* Vol. 89, 1988, pp. 5739–5746.
5. Seijo, L. and Barandiaran, Z. Self-consistent embedded clusters: building block equations for localized orthogonal orbitals, *J Math Chem.,* Vol. 10, 1992, pp. 41–56.
6. Seijo, L. and Barandiaran, Z. Application of the group-function theory to the field of materials science, *Int J Quantum Chem.,* Vol. 60, 1996, pp. 617–634.
7. Mejias, J. A. and Sanz, J. F. Compact model potentials for ab initio embedded cluster calculations. Part I. Basic Formulation, *J Chem Phys.,* Vol. 102, 1995, pp. 327–336. Unrestricted compact model potentials for ab initio embedded cluster calculations: Magnetic interactions in $KNiF_3$, *J Chem Phys.,* Vol. 102, 1995, pp. 850–858.
8. Anderson, P. W. Self-consistent pseudopotentials and ultra-localized functions for energy bands, *Phys Rev Lett.,* Vol. 21, 1968, pp. 13–16.
9. Adams, W. H. On the solution of the Hartree–Fock equation in terms of localized orbitals, *J Chem Phys.,* Vol. 34, 1961, pp. 89–102.
10. Adams, W. H. Orbital theories of electronic structure, *J Chem Phys.,* Vol. 37, 1962, pp. 2009–2018.
11. Adams, W. H. Orbital theories of electronic structure. II. Molecularly invariant orbitals, *J Chem Phys.,* Vol. 42, 1965, pp. 4030–4038.
12. Gilbert, T. L. Self-consistent equations for localized orbitals in polyatomic systems. In: *Molecular Orbitals in Chemistry, Physics and Biology.* New York and London: Academic Press, 1964, pp. 405–420.

13. Gilbert, T. L. Selection of self-consistent-field orbitals, *J Chem Phys.,* Vol. 60, 1974, pp. 1789–1791.
14. Szasz, L. *Pseudopotential Theory of Atoms and Molecules.* New York: John Wiley, 1985.
15. Weeks, J. D. and Rice, S. A. Use of pseudopotentials in atomic-structure calculations, *J Chem Phys.,* Vol. 49, 1968, pp. 2741–2755.
16. Ewig, C. S. and Van Wazer, J. R. On pseudopotential and effective-potential SCF theory and its application to compounds of heavy elements, *J Chem Phys.,* Vol. 63, 1975, pp. 4035–4041.
17. Kahn, L. R., Baybutt, P. and Truhlar, D. G. Ab initio effective core potentials: Reduction of all-electron molecular structure calculations to calculations involving only valence electrons, *J Chem Phys.,* Vol. 65, 1976, pp. 3826–3853.
18. Shidlovskaya, E. K. Rigorous approach to the construction of pseudopotential from crystalline environment in embedded molecular cluster model, *Latvian Journal of Physics and Technical Sciences,* No. 4, 1996, pp. 57–82.
19. Shidlovskaya, E. K. Improved embedded molecular cluster model, *Int J Quantum Chem.,* Vol. 89, 2002, pp. 349–370.
20. Shidlovskaya, E. K. Problem of Cluster Embedding in Crystalline Lattice, *Computer Modelling and New Technologies,* Vol. 10**,** No 4, 2006, pp. 17–28.
21. Löwdin, P.-O. Quantum theory of many-particle systems. II. Study of the ordinary Hartree–Fock approximation, *Phys Rev.,* Vol. 97, 1955, pp. 1490–1508.
22. Löwdin, P.-O. On the non-orthogonality problem connected with the use of atomic wave functions in the theory of molecules and crystals, *J Chem Phys.,* Vol. 18, 1950, pp. 365–375.
23. Stoll, H., Wagenblast, G. and Preuss, H. On the Hartree–Fock theory of local regions in molecules, *J Am Chem Soc.,* Vol. 100, 1978, pp. 7742–7743.
24. Stoll, H., Wagenblast, G. and Preuss, H. On the use of local basis sets for localized molecular orbitals, *Theor Chim Acta.,* Vol. 57, 1980, pp. 169–178.
25. Shidlovskaya, E. K. Embedded Molecular Cluster Model with Improved Boundary Conditions, *Latvian Journal of Physics and Technical Sciences,* No. 2, 1997, pp. 13–32.

Appendix

When we divide quantum system on two subsystems (cluster and the rest of system in our case) matrix of one-electron wave functions overlaps and its inverse may be written in the block form:

$$S = \begin{pmatrix} S_c & S_{cr} \\ S_{rc} & S_r \end{pmatrix}, \qquad S^{-1} = Q = \begin{pmatrix} Q^c & Q^{cr} \\ Q^{rc} & Q^r \end{pmatrix}.$$

According to the definition of the inverse matrix, $QS = I$, where I is unit matrix. Write this equality in the block form:

$$Q^c S_c + Q^{cr} S_{rc} = I_c, \qquad \text{(A1)} \qquad Q^c S_{cr} + Q^{cr} S_r = 0, \qquad \text{(A2)}$$

$$Q^{rc} S_c + Q^r S_{rc} = 0, \qquad \text{(A3)} \qquad Q^{rc} S_{cr} + Q^r S_r = I_r. \qquad \text{(A4)}$$

From (A2) and (A3) we obtain

$$Q^{cr} = -Q^c S_{cr} S_r^{-1}, \qquad \text{(A5)} \qquad Q^{rc} = -Q^r S_{rc} S_c^{-1}. \qquad \text{(A6)}$$

Substituting (A5) in (A1) we get

$$Q^c S_c - Q^c S_{cr} S_r^{-1} S_{rc} = I_c.$$

Therefore

$$Q^c = \left(S_c - S_{cr} S_r^{-1} S_{rc}\right)^{-1}. \qquad \text{(A7)}$$

In the similar way, substituting (A6) in (A4), we come to

$$Q^r = \left(S_r - S_{rc} S_c^{-1} S_{cr}\right)^{-1}. \qquad \text{(A8)}$$

On the other hand, according to the definition of the inverse matrix, $SQ = I$. Write this equality in the block form:

$$S_c Q^c + S_{cr} Q^{rc} = I_c, \qquad S_c Q^{cr} + S_{cr} Q^r = 0, \qquad \text{(A9)}$$

$$S_{rc} Q^c + S_r Q^{rc} = 0, \qquad \text{(A10)} \qquad S_{rc} Q^{cr} + S_r Q^r = I_r.$$

From (A9) and (A10) we obtain

$$Q^{cr} = -S_c^{-1} S_{cr} Q^r, \qquad \text{(A11)} \qquad Q^{rc} = -S_r^{-1} S_{rc} Q^c. \qquad \text{(A12)}$$

Substituting (A11) in (A1) we have

$$Q^c S_c - S_c^{-1} S_{cr} Q^r S_{rc} = I_c.$$

Therefore

$$Q^c = S_c^{-1} + S_c^{-1} S_{cr} Q^r S_{rc} S_c^{-1}. \qquad \text{(A13)}$$

In a similar way, substituting (A12) in (A4) we come to

$$Q^r = S_r^{-1} + S_r^{-1} S_{rc} Q^c S_{cr} S_r^{-1}. \qquad \text{(A14)}$$

Collecting these results we finally have

$$Q^c = \left(S_c - S_{cr} S_r^{-1} S_{rc}\right)^{-1} = S_c^{-1} + S_c^{-1} S_{cr} Q^r S_{rc} S_c^{-1};$$

$$Q^{cr} = -Q^c S_{cr} S_r^{-1} = -S_c^{-1} S_{cr} Q^r;$$

$$Q^{rc} = -Q^r S_{rc} S_c^{-1} = -S_r^{-1} S_{rc} Q^c;$$

$$Q^r = \left(S_r - S_{rc} S_c^{-1} S_{cr}\right)^{-1} = S_r^{-1} + S_r^{-1} S_{rc} Q^c S_{cr} S_r^{-1}.$$

Consider wave functions of the cluster, which are linearly independent with those of the frozen rest of our system. Without loss of generality they may be expressed as follows:

$$\left|\psi_i\right\rangle = \left|\phi_i\right\rangle + \sum_{j \in r} \left|\varphi_j\right\rangle a_{ji}, \quad i \in \mathrm{c}, \qquad \text{(A15)}$$

where

$\left|\varphi_j\right\rangle$, $j \in$ r, are wave functions of the rest of system, they are not mutually orthogonal, $\left\langle \varphi_i \middle| \varphi_j \right\rangle = \left(S_r\right)_{ij}$;

$\left|\phi_i\right\rangle$, $i \in$ c, are orthogonal to the rest of system components of the cluster wave functions, $\left\langle \phi_i \middle| \varphi_j \right\rangle = 0$, they are linearly independent but in general case are not mutually orthogonal, $\left\langle \phi_i \middle| \phi_j \right\rangle = B_{ij}$;

coefficients a_{ji} describe overlaps between the cluster and the rest of system wave functions.

Using this expansion, we get the following expressions for the wave functions overlap matrix S for our system (cluster + the rest of system):

$$S = \begin{pmatrix} S_c & S_{cr} \\ S_{rc} & S_r \end{pmatrix} = \begin{pmatrix} B + A^+ S_r A & A^+ S_r \\ S_r A & S_r \end{pmatrix}, \qquad \text{(A16)}$$

where A is matrix of coefficients a_{ji} in the expansion (A15) for the cluster wave functions.

For the inverse matrix $Q = S^{-1}$, substituting (A16) in formulas (A7), (A5), (A12) and (A14), we finally get

$$S^{-1} = Q = \begin{pmatrix} Q^c & Q^{cr} \\ Q^{rc} & Q^r \end{pmatrix} = \begin{pmatrix} B^{-1} & -B^{-1} A^+ \\ -AB^{-1} & S_r^{-1} + AB^{-1} A^+ \end{pmatrix}. \qquad \text{(A17)}$$

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CORRECTIVE MAINTENANCE AND RELIABILITY ASSOCIATED COST ESTIMATION OF AGING MULTI-STATE SYSTEMS

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This paper considers corrective maintenance contracts for aging air conditioning systems, operating under varying weather conditions. Aging is treated as an increasing failure rate. The system can fall into unacceptable states for two reasons: through performance degradation because of failures or through an increase in demand of cold. Each residence in acceptable state, each repair and each entrance to an unacceptable state are associated with a corresponding cost. A procedure for computing this reliability associated cost is based on the Markov reward model for a non-homogeneous Poisson process. By using this model an optimal maintenance contract that maximizes the total expected cost may be found. A numerical example for a real world air conditioning system is presented to illustrate the approach.

Keywords*: corrective maintenance, reliability associated cost, aging, multi-state system, Markov reward model*

1. Introduction

Many technical systems are subjected to aging and degradation during their lifetime. Most of these systems are repairable. Maintenance and repair problems have been widely investigated in the literature. Barlow and Proshan [3], Gertsbakh [4], Pham and Wang [16], Wang [19] survey and summarize theoretical developments and practical applications of maintenance models.

Maintenance strategies addressed in most previous research works have been developed for improving reliability of aging binary-state systems or products. There is relatively limited number of research works focused on the maintenance strategies for aging Multi-state System (MSS). A heuristic approach has been proposed by Nourelfath and Ait-Kadi [14] for the optimisation of series–parallel MSSs when the maintenance resources are limited. Hsieh and Chiu [6] have proposed an optimal maintenance policy for a multi-state deteriorating standby system, by determining the optimal number of standby components and the optimal state in which deteriorating components shall be replaced. Nourelfath and Dutuit [15] have proposed a combined approach to solve the redundancy optimisation problem for multi-state systems under repair policies. The problem of imperfect preventive maintenance optimisation was considered for ageing MSS by Levitin and Lisnianski [9].

With the increasing complexity of the systems, only specially trained staff with specialized equipment can provide system service. In this case, maintenance service is provided by an external agent and the owner is considered as a customer of the agent for maintenance service (Pongpech and Murthy [17]). The maintenance outsourcing has been discussed by Jaturonnatee et al. [8] and Huang et al. [7]. Murthy and Asgharizadeh [13] have proposed a model to determine the optimal pricing strategy, the number of customers to service and the number of service channels for a monopolist service agent providing the maintenance service. The maintenance contract models have been studied by Bai and Pham [2], which discussed discounted warranty cost models for repairable series systems. The maintenance contract selection and spares provisioning planning based on the multi-criteria decision models has been discussed by Almeida [1]. Tarakci at al. [18] considered a manufacturer who has a process with an increasing failure rate over time. In order to improve the process performance, preventive maintenance and corrective maintenance are outsourced to an external contractor. Authors recommend to use the incentive contracts to induce the contractor to select the maintenance policy that optimises the total profit of the manufacturer and contractor.

Most of papers, that consider the maintenance contract selection, assume that the manufacturing process is binary-state. However the methods for the optimal maintenance contract planning for a multi-state aging system in a life cycle period till now have not been comprehensively developed.

This paper presents a case study where an aging air conditioning system with minimal repair is considered. Aging is considered a process which results in an age-related increase of the failure rate. The Markov reward model is built for computing the reliability associated cost, accumulated during the system's life span. By using the model a corrective maintenance contract with maximum reliability associated cost can be defined from the set of different contracts available in the market. The approach is based on the Non-Homogeneous Markov Reward Model. The main advantage of the suggested approach is that it can be easily implemented in practice by reliability engineers.

2. Problem Formulation and Model Description

2.1. Reliability Associated Cost and Corrective Maintenance Contracts

We will define the Reliability Associated Cost (RAC) as the difference between total income from system using and total cost incurred by the user in operations and maintenance of the system during its lifetime. Therefore,

$$RAC = US - OC - RC - PC, \quad (1)$$

where

- US is income (reward) from system using.
- OC is the system operating cost accumulated during the system lifetime;
- RC is the repair cost incurred by the user in operating and maintaining the system during its lifetime;
- PC is a penalty cost, accumulated during system life time, which was paid when the system failed.

Let T be the system lifetime. During this time the system may be in acceptable states (system functioning) or in unacceptable ones (system failure). After any failure, a corresponding repair action is performed and the system returns to one of the previously acceptable states.

A Maintenance Contract is an agreement between the repair team and the system's owner. The Maintenance Contract defines possible Maintenance Contract level, mean repair time and repair rate. Repair cost depends on repair time and, so, it corresponds to a maintenance contract level.

The problem is to find the expected reliability associated cost corresponding to each maintenance contract and choose the contract, maximizing this cost. According to the suggested approach, this cost is represented by the total expected reward, calculated via a specially developed Markov reward model.

2.2. Markov Reward Model for Aging System

Markov reward model was first introduced by Howard [5], and applied to multi-state system (MSS) reliability analysis by Lisnianski and Levitin [12].

We suppose that the Markov model for the system has K states that may be represented by a state space diagram as well as transitions between states. Intensities a_{ij}, $i, j = 1,...,K$ of transitions from state i to state j are defined by corresponding failure and repair rates.

It is assumed that while the system is in any state i during any time unit, some payment r_{ii} will be made. It is also assumed that if there is a transition from state i to state j the amount r_{ij} will by paid for each transition. The amounts r_{ii} and r_{ij} are called rewards. The objective is to compute the total expected reward accumulated from $t = 0$, when the system begins its evolution in the state space, up to the time $t = T$ under specified initial conditions.

Let $V_j(t)$ be the total expected reward accumulated up to time t, if the system begins its evolution at time $t = 0$ from state j. According to Howard [5], the following system of differential equations must be solved in order to find this reward:

$$\frac{dV_j(t)}{dt} = r_{jj} + \sum_{\substack{i=1 \\ i \neq j}}^{K} a_{ij} r_{ij} + \sum_{i=1}^{K} a_{ij} V_i(t), \quad j = 1,2,...,K \quad (2)$$

The system (2) should be solved under specified initial conditions: $V_j(0) = 0,\ j = 1, 2, ..., K.$

For an aging system, its failure rate $\lambda(t)$ increases with age. In the case of minimal repair, the intensities $a_{ij},\ i, j = 1, ..., K$ of transitions from state *i* to state *j* corresponding to failures are dependent on time. The total expected reward can be found from differential equations (2), by substitution of formulae for $\lambda(t)$ instead of corresponding a_{ij} values.

3. Numerical Example

3.1. The System Description

Consider an air conditioning system, used around the clock in varying temperature conditions and consists of two air conditioners, main and reserved. The main air conditioner is aging multi-state cold generating unit with 4 different levels: the first level of perfect functioning, the second level with reduced capacity (partial filter obstruction), the third level with complete failure (full filter obstruction) and the fourth level with complete failure (another reasons). The reserved air conditioner may be only in two states: perfect functioning or full failure.

The work schedule of the system is as follows. For regular temperature conditions the main air conditioner must be on-line. For peak temperature conditions if the main unit is in the level with reduced capacity, in addition to main air conditioner the reserved one must be on-line.

The state-space diagram for this system is presented on Figure 1. States 1–4 correspond to regular conditions and states 5–9 correspond to peak conditions. States 4 and 8 correspond to perfect functioning of the main air conditioner. States 3 and 7 corresponds to the reduced capacity level of the main conditioner. If the system enters to the state 7 the reserved air conditioner starts immediately his functioning. States 2 and 6 corresponds to complete failure of the main air conditioner because full filter obstruction and states 1 and 5 corresponds to complete failure because another reasons. State 9 corresponds to failure of the reserved air conditioner.

As was written above, technical requirements demand that the main on-line air conditioner are needed under regular conditions and additional reserved one in peak condition, so that there are four acceptable states – states 3–4 and states 7–8, and 5 unacceptable states: states 1–2, states 5–6 and state 9.

Aging is indicated as increasing failure rate functions: $\lambda_{41}(t) = 1 + 0.9t$ year^{-1}, $\lambda_{31}(t) = 1 + 0.9t$ year^{-1}, $\lambda_{85}(t) = 1 + 0.9t$ year^{-1} and $\lambda_{75}(t) = 1 + 0.9t$ year^{-1}. Other failure rates are constant: $\lambda_{43} = \lambda_{32} = \lambda_{87} = \lambda_{76} = 4$ year^{-1} and $\lambda_{79} = 1$ year^{-1}.

Repair rates are the following: $\mu_{24} = \mu_{68} = 700$ year^{-1}, $\mu_{97} = 365$ year^{-1}. $\mu_{14} = \mu_{58} = 2000 \div 200$ year^{-1} (see Table 1).

Following Lisnianski [10], the variable demand, representing variable weather conditions, may be described as a continuous time Markov chain with 2 levels. The first level represents a regular temperature conditions and the second level represents peak temperature conditions. The cycle time is $T_c = 24$ hours and the mean duration of the peak is $t_d = 9$ hours. The transition intensities of the model can be obtained as

$$\lambda_d = \frac{1}{T_c - t_d} = 0.066 hours^{-1} = 584 year^{-1},\ \lambda_N = \frac{1}{t_d} = 0.111 hours^{-1} = 972 year^{-1}.$$

We denote:

C_{us} – is the income (reward) from system using.

C_{op} – is the system operations cost accumulated during the system lifetime.

C_r^m – is the repair cost paid for every order of the external maintenance team;

C_r – is the repair cost incurred by the user maintaining the reserved air conditioner;

C_p – is a penalty cost, which is paid when system failed.

Service agents can suggest 10 different Corrective Maintenance Contracts, available in the market. Each contract *m* is characterized by repair rate and corresponding repair cost (per repair) C_r^m as presented in the Table 1.

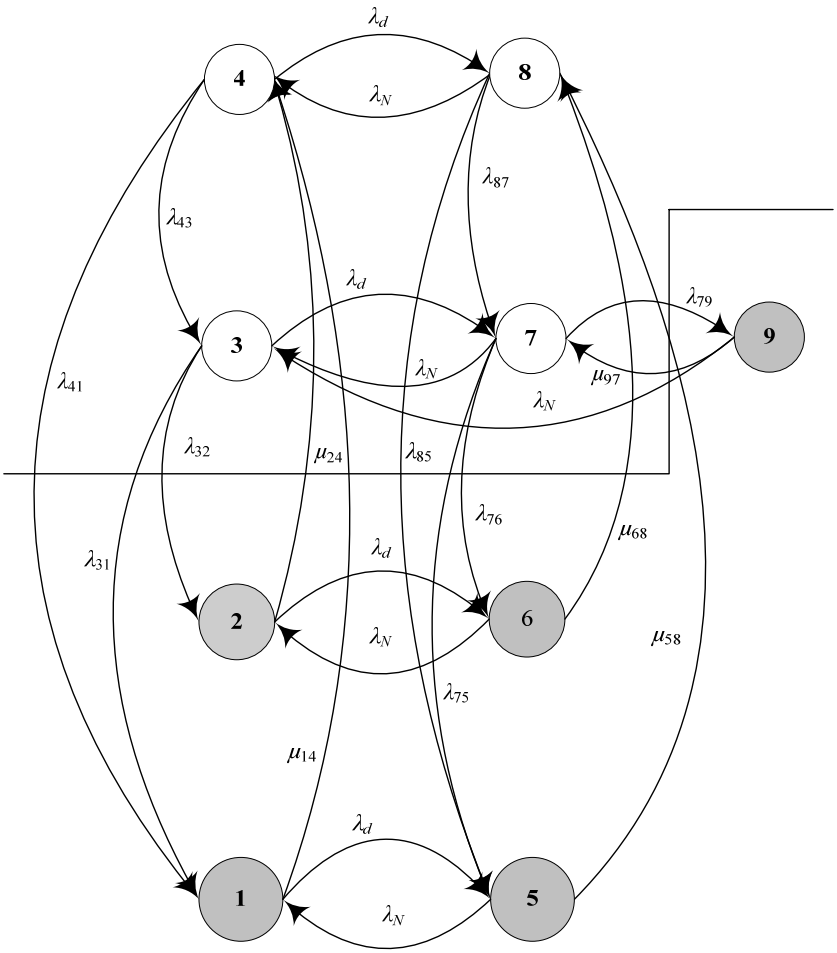

Figure 1. The state-space diagram for the air-conditioning system with reserve

Table 1. Maintenance Contract Characteristics

Maintenance Contract	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**
Repair rate (year^{-1})	2000	1800	1600	1400	1200	1000	800	600	400	200
Mean Repair Time (days)	0.18	0.21	0.23	0.26	0.30	0.37	0.46	0.61	0.91	1.83
Repair cost ($ per repair)	1453	1143	899	708	557	438	344	270	213	167

The income (reward) from system using C_r^m is equal \$180000 per year. The repair cost incurred by the user C_r, is equal to \$50 per repair. The operation cost C_{op}, is equal to \$7200 per year. The penalty cost C_p, which is paid when the system fails, is equal to \$13140 per failure.

3.2. The Markov Reward Model for the System

The transition intensity matrix for the system is as shown in (3).

$$a=\begin{vmatrix} a_{11} & 0 & 0 & \mu_{14} & \lambda_d & 0 & 0 & 0 & 0 \\ 0 & a_{22} & 0 & \mu_{24} & 0 & \lambda_d & 0 & 0 & 0 \\ \lambda_{31}(t) & \lambda_{32} & a_{33} & 0 & 0 & 0 & \lambda_d & 0 & 0 \\ \lambda_{41}(t) & 0 & \lambda_{43} & a_{44} & 0 & 0 & 0 & \lambda_d & 0 \\ \lambda_N & 0 & 0 & 0 & a_{55} & 0 & 0 & \mu_{58} & 0 \\ 0 & \lambda_N & 0 & 0 & 0 & a_{66} & 0 & \mu_{68} & 0 \\ 0 & 0 & \lambda_N & 0 & \lambda_{75}(t) & \lambda_{76} & a_{77} & 0 & \lambda_{79} \\ 0 & 0 & 0 & \lambda_N & \lambda_{85}(t) & \lambda_{87} & 0 & a_{88} & 0 \\ 0 & 0 & \lambda_N & 0 & 0 & 0 & \mu_{97} & 0 & a_{99} \end{vmatrix}, \tag{3}$$

where

$$a_{11}=-(\mu_{14}+\lambda_d), \quad a_{44}=-(\lambda_{41}(t)+\lambda_{43}+\lambda_d), \quad a_{77}=-(\lambda_{75}(t)+\lambda_{76}+\lambda_{79}+\lambda_N),$$
$$a_{22}=-(\mu_{24}+\lambda_d), \quad a_{55}=-(\mu_{58}+\lambda_N), \quad a_{88}=-(\lambda_{85}(t)+\lambda_{87}+\lambda_N),$$
$$a_{33}=-(\lambda_{31}(t)+\lambda_{32}+\lambda_d), \quad a_{66}=-(\mu_{68}+\lambda_N), \quad a_{99}=-(\mu_{97}+\lambda_N).$$

To calculate the total expected reward, the reward matrix for the system is built in the following manner (see Lisnianski and Levitin [12] and Lisnianski et al. [11]).

If the system is in states $3, 4, 7$ and 8, the income (reward) from system using minus the operation cost associated with use of air conditioners, should be received during any time unit.

The transitions $3\to1$, $4\to1$, $7\to5$, $8\to5$ and $7\to9$ are associated with the entrance to unacceptable states and rewards associated with this transitions are the penalty.

The transitions $1\to4$, $5\to8$, $9\to3$ and $9\to7$ are associated with the repair of the air conditioner, provided by external team, and the reward associated with this transition is the repair cost paid for every order of the external maintenance team. The transitions $2\to3$ and $6\to7$ are associated with the filter repair, and the reward is the cost of this repair. The reward matrix for the system of air conditioners is as shown in (4).

$$r=\begin{vmatrix} 0 & 0 & 0 & -C_r^m & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -C_r & 0 & 0 & 0 & 0 & 0 \\ -C_p & -C_p & C_{us}-C_{op} & 0 & 0 & 0 & 0 & 0 & 0 \\ -C_p & 0 & 0 & C_{us}-C_{op} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -C_r^m 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -C_r 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & C_{us}-C_{op} & 0 & -C_p \\ 0 & 0 & 0 & 0 & -C_p & 0 & 0 & C_{us}-C_{op} & 0 \\ 0 & 0 & -C_r^m & 0 & 0 & 0 & -C_r^m & 0 & 0 \end{vmatrix} \tag{4}$$

Taking into consideration the transition intensity matrix (3), the system of differential equations that defines the Markov reward model for the air conditioning system for the calculation of the total expected reward, may be written as shown in (5).

The system is solved under initial conditions: $V_i(0) = 0,\ i = 1,2,...,9$ using MATLAB®, the language of technical computing.

$$
\begin{aligned}
\frac{dV_1(t)}{dt} &= -C_r^m \mu_{14} - (\mu_{14} + \lambda_d)V_1(t) + \mu_{14}V_1(t) + \lambda_d V_5(t) \\
\frac{dV_2(t)}{dt} &= -C_r \mu_{24} - (\mu_{24} + \lambda_d)V_2(t) + \mu_{24}V_4(t) + \lambda_d V_6(t) \\
\frac{dV_3(t)}{dt} &= C_{us} - C_{op} - C_p(\lambda_{31} + \lambda_{32}) + \lambda_{31}V_1(t) + \lambda_{32}V_2(t) - (\lambda_{31} + \lambda_{32} + \lambda_d)V_3(t) + \lambda_d V_7(t) \\
\frac{dV_4(t)}{dt} &= C_{us} - C_{op} - C_p\lambda_{41} + \lambda_{41}V_1(t) + \lambda_{43}V_3(t) - (\lambda_{41} + \lambda_{43} + \lambda_d)V_4(t) + \lambda_d V_8(t) \\
\frac{dV_5(t)}{dt} &= -C_r^m \mu_{58} + \lambda_N V_1(t) - (\mu_{58} + \lambda_N)V_5(t) + \mu_{58}V_8(t) \\
\frac{dV_6(t)}{dt} &= -C_r^m \mu_{68} + \lambda_N V_2(t) - (\mu_{68} + \lambda_N)V_6(t) + \mu_{68}V_8(t) \\
\frac{dV_7(t)}{dt} &= C_{us} - C_{op} - C_p\lambda_{79} + \lambda_N V_3(t) + \lambda_{75}V_5(t) + \lambda_{76}V_6(t) - (\lambda_{75} + \lambda_{76} + \lambda_{79} + \lambda_N)V_7(t) + \lambda_{79}V_9(t) \\
\frac{dV_8(t)}{dt} &= C_{us} - C_{op} - C_p\lambda_{85} + \lambda_N V_4(t) + \lambda_{85}V_5(t) + \lambda_{87}V_7(t) - (\lambda_{85} + \lambda_{87} + \lambda_N)V_8(t) \\
\frac{dV_9(t)}{dt} &= -C_r^m \mu_{97} + \lambda_N V_3(t) + \mu_{97}V_7(t) - (\mu_{97} + \lambda_N)V_9(t)
\end{aligned}
\tag{5}
$$

4. Calculation Results

By using the suggested method one will find the best maintenance contract level *m* that provides a maximum of Reliability Associated Cost during system lifetime. Figure 2 shows the expected Reliability Associated Cost for $T = 1$ years as a function of the Maintenance Contract Level (m). The eighth level (m = 8), which provides the maximum expected reliability associated cost ($140780) for the system, corresponds to a mean repair time of 0.61 days. Choosing a more expensive Maintenance Contract Level, we pay an additional payment to the repair team. Choosing a less expensive one, we pay more for penalties because of transitions to unacceptable states.

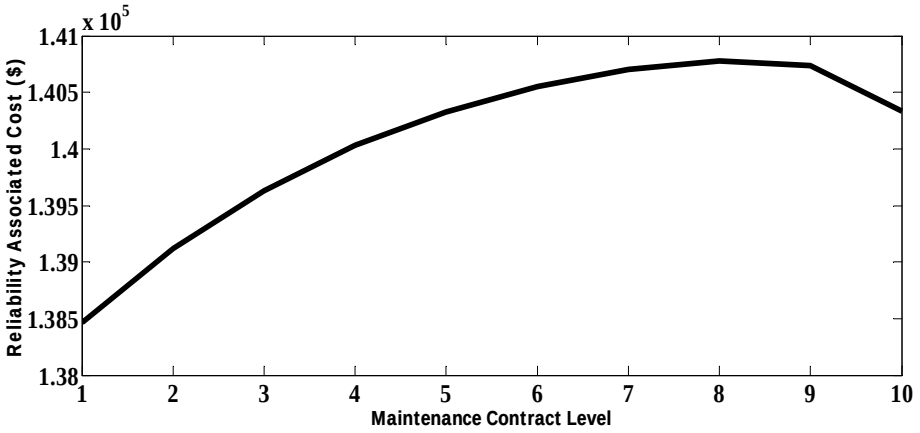

Figure 2. The expected Reliability Associated Cost vs. Maintenance Contract Level

Conclusions

The case study for the estimation of expected reliability associated cost accumulated during system lifetime is considered for an aging system under minimal repair. The approach is based on application of a special Markov reward model, well formalized and suitable for practical application in reliability engineering. The optimal corrective maintenance contract (m = 8), which provides maximum expected reliability associated cost ($140780), was found.

References

1. Almeida, de A. T. Multicriteria Decision Making on Maintenance: Spares and Contract Planning, *European Journal of Operational Research,* Vol. 129, 2001, pp. 235–241.
2. Bai, J., Pham, H. Discounted Warranty Cost of Minimally Repaired Series Systems, *IEEE Transaction on Reliability,* Vol. 53, No 1, 2004, pp. 37–42.
3. Barlow, R. E., Proshan, F. *Statistical Theory of Reliability and Life Testing*. New-York: Holt, Rinehart and Winston, 1975.
4. Gertsbakh, I. *Reliability Theory with Applications to Preventive Maintenance*. Berlin: Springer-Verlag, 2000.
5. Howard, R. *Dynamic Programming and Markov Processes*. Cambridge, Massachusetts: MIT Press, 1960.
6. Hsieh, C., Chiu, K. Optimal Maintenance Policy in a Multistate Deteriorating Standby System, *European Journal of Operational Research,* Vol. 141, No 3, 2002, pp. 689–698.
7. Huang, H. Z., Liu, Z. J., Murthy, D. N. P. Optimal Reliability, Warranty and Price for New Products, *IIE Transactions,* Vol. 39, 2007, pp. 819–827.
8. Jaturonnatee, J., Murthy, D. N. P., Boondiskulchok, R. Optimal Preventive Maintenance of Leased Equipment with Corrective Minimal Repairs, *European Journal of Operational Research,* Vol. 174, No 1, 2006, pp. 201–215.
9. Levitin, G., Lisnianski, A. Joint Redundancy and Maintenance Optimization for Multi-state Series-parallel Systems, *Reliability Engineering and System Safety,* Vol. 64, No 1, 1998, pp. 33–42.
10. Lisnianski, A. The Markov Reward Model for a Multi-state System Reliability Assessment with Variable Demand, *Quality Technology & Quantitative Management,* Vol. 4, No 2, 2007, pp. 265–278.
11. Lisnianski, A., Frenkel, I., Khvatskin, L., Ding, Yi. Maintenance contract assessment for aging system, *Quality and Reliability Engineering International,* Vol. 24, 2008, pp. 519–531.
12. Lisnianski, A., Levitin, G. *Multi-state System Reliability. Assessment, Optimization and Applications.* Singapore, London, NJ: World Scientific, 2003.
13. Murthy, D. N. P., Asgharizadeh, E. Optimal decision Making in a Maintenance Service Operation, *European Journal of Operational Research,* Vol. 116, 1999, pp. 259–273.
14. Nourelfath, M., Ait-Kadi, D. Optimization of series–parallel multi-state systems under maintenance policies, *Reliability Engineering & System Safety,* Vol. 92, No 12, 2007, pp. 1620–1626.
15. Nourelfath, M., Dutuit, Y. A combined approach to solve the redundancy optimization problem for multi-state systems under repair policies, *Reliability Engineering & System Safety,* Vol. 86, No 3, 2004, pp. 205–213.
16. Pham, H., Wang, H. Imperfect Maintenance, *European Journal of Operational Research,* Vol. 95, 1996, pp. 425–438.
17. Pongpech, J., Murthy, D. N. P. Optimal Periodic Preventive Maintenance Policy for Leased Equipment, *Reliability Engineering and System Safety,* Vol. 91, No 7, 2006, pp. 772–777.
18. Tarakci, H., Tang, K., Moskowitz, H., Plante, R. Incentive maintenance outsourcing contracts for channel coordination and improvement. *IIE Transactions,* Vol. 38, 2006, pp. 671–684.
19. Wang, H. A Survey of Maintenance Policies of Deteriorating Systems, *European Journal of Operational Research,* Vol. 139, 2002, pp. 469–489.

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PROPERTIES OF GUARANTEED REACHABLE SETS FOR LINEAR DYNAMIC SYSTEMS UNDER UNCERTAINTIES WITH INTERMEDIATE CORRECTION POINTS

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In the paper we consider the problem of investigation and constructive description of the reachable sets for linear dynamic systems under unknown but bounded uncertainties over feasible controls that are allowed to be corrected in a given set of correction moments. It is showed that construction of the reachable sets under considered class of feasible uncertainties can be reduced to solving a multilevel min-max optimisation problem with respect to finite dimensional decision variables.

It is proved that adding one new correction moment leads to an extension of the set of system states that can be guaranteed reached at a terminal moment from a given initial position over a feasible control strategy. Numerical example illustrates theoretical results. Some rules for construction external and internal approximations for the reachable sets are discussed.

Keywords: *reachability set, control system, bounded uncertainties*

1. Introduction

One of the central problems in mathematical optimal control theory is the problem of constructive description and determination of the reachability set for a given controlled system, i.e. the set of all system states that can be reached at a final moment from a given initial state with some feasible control function. There exists a wide range of literature devoted to investigation and construction of the reachability sets [1–5]. Such investigations are important both form theoretical and practical points of view since they allow us to evaluate potentialities of different dynamic system. For systems with uncertainties, the reachability sets give an opportunity to evaluate system states spread under these uncertainties.

The problem of computation of the reachability set can be interpreted as a special problem of theory of differential games. In such problem statement, both control and uncertainty are considered as actions of the first and the second players respectively but for all that the second player has no certain objects. However, if one follows a guaranteed approach then the aim of the second is to do damage to the first player [2, 4].

In many practical problems, the exact determination of the reachability set is very difficult task.

Therefore, in many applications, the exact reachability set is replaced by internal or external approximation which has more simple structure, for example by some polyhedron or ellipsoid. At present there is a number of methods for constructing approximation of reachable sets of dynamic controlled systems. In particular, much attention is paid to ellipsoidal approximations [2–5].

In this paper, we investigate properties of the reachable sets for dynamic controlled systems with uncertainties. It is supposed that control function can be corrected in some given moments on the base of available information about current system state. It is well-known [6–8] that these allowed control corrections lead to extended reachable set compared to approaches that do not use control corrections. The price that must be paid for this benefit is that the computational demands for solving corresponding multilevel min-max optimisation problems may be very high. In the paper we show that arising min-max optimisation problem with respect to functional decision variables may be reduce to a multilevel min-max with respect to finite dimensional decision variables. This allows us to give constructive description of the reachable set and investigate its properties. Theoretical results are illustrated by a numerical example.

2. Problem Statement. Definitions

Consider a dynamic system that behaviour is described by the following system of ordinary differential equations

$$\dot{z}(t) = Az(t) + bu(t) + gw(t),\ t \in T = [0, t_*],\ z(0) = z_0, \tag{1}$$

where $z(t) \in R^n$ is a system state, $u(\cdot) = (u(t), t \in T) \in U$, is a scalar control function, $w(\cdot) = (w(t),\ t \in T) \in W$ is unknown disturbance, matrix $A \in R^{n \times n}$, and vectors $b, g \in R^n$, and moments

t_0, t_* are considered to be given. The set of feasible controls U and the set of feasible disturbances W are defined as follows:

$$U = U(T) = \{u(\cdot) = (u_s(\cdot), s = 1,..., N+1): u_s(\cdot) \in U_s,\ s = 1,..., N+1\},$$

$$W = W(T) = \{w(\cdot) = (w_s(\cdot), s = 1,..., N+1): u_s(\cdot) \in W_s,\ s = 1,..., N+1\},$$

$$U_s = \{u_s(\cdot) = (u(t), t \in T_s) \in L_2(T_s): \int_{T_s} u^2(t)dt \le r_s\},$$

$$W_s = \{u_s(\cdot) = (w(t), t \in T_s) \in L_2(T_s): \int_{T_s} w^2(t)dt \le v_s\},$$

where $T_s = [t_{s-1}, t_s]$, numbers $r_s >, v_s > 0$, $s = 1,..., N+1$, are given, t_s, $s = 0,..., N+1$, are given instances of time from the control interval T:

$$0 = t_0 < t_1 < ... < t_N < t_{N+1} = t_*. \tag{2}$$

Denote by $z(t \mid x, \tau, u(\cdot), w(\cdot)), t \ge \tau$, the trajectory of the system
$\dot{z}(t) = Az(t) + bu(t) + gw(t), t \ge \tau, z(\tau) = x,$
generated by an initial state $z(\tau) = x,$ by a control $u(\cdot)$ and by a disturbance $w(\cdot)$.

Pair (z_*, τ_*) of n-vector z_* and a moment $\tau_* \in T$ is called a position of system (1). We say that system is in a position (z_*, τ_*) if at the moment τ_* system state is z_*.

Let us consider some subset of time instances from a given set (2)

$$\tau_i = t_{m_i}, i = 0,..., i_*,\ m_0 = 0 < m_1 < m_2 < .... < m_{i_*} < N+1 = m_{i_*+1}. \tag{3}$$

For $i = 0,1,..., i_*,$ denote

$$I_i = \{m_i + 1, m_i + 2,..., m_{i+1}\},$$

$$U^{(i)} = \{u^{(i)}(\cdot) = (u(t), t \in [\tau_i, \tau_{i+1}]) = (u_s(\cdot), s \in I_i): u_s(\cdot) \in U_s, s \in I_i\},$$

$$W^{(i)} = \{w^{(i)}(\cdot) = (w(t), t \in [\tau_i, \tau_{i+1}]) = (w_s(\cdot), s \in I_i): w_s(\cdot) \in W_s, s \in I_i\}.$$

Given $\mu_* > 0,\ Q_* = Q_*^T \dot{>} 0,\ Q_* \in R^{n \times n}$, denote $B(x \mid \mu_*, Q_*) = \{z \in R^n: \|z - x\|_{Q_*}^2 \le \mu_*\}$.

Definition 1. *A system state $x \in R^n$ is said to be (μ_*, Q_*) – guaranteed reachable (at the terminal moment $t = t_*$) from a position (z_{i_*}, τ_{i_*}), $z_{i_*} \in R^n$, $0 \le \tau_{i_*} < t_*$, if there exists a control $u^{(i_*)}(\cdot) \in U^{(i_*)}$, such that $Z_{i_*}(z_{i_*}, u^{(i_*)}(\cdot)) \subset B(x \mid \mu_*, Q_*)$.*

Here and in what follows $Z_i(z_i, u^{(i)}(\cdot)) = \{z = z(\tau_{i+1} \mid z_i, \tau_i, u^{(i)}(\cdot), w^{(i)}(\cdot)): w^{(i)}(\cdot) \in W^{(i)}\}$.

Definition 2. *A system state $x \in R^n$ is said to be (μ_*, Q_*) – guaranteed reachable (at the terminal moment $t = t_*$) form a position $(z_{i_*-1}, \tau_{i_*-1})$, $z_{i_*-1} \in R^n$, $0 \le \tau_{i_*-1} < \tau_{i_*}$, subject to one correction moment τ_{i_*}, if there exists a control $u^{(i_*-1)}(\cdot) \in U^{(i_*-1)}$, such that the state x is (μ_*, Q_*) – guaranteed reachable from all positions (z, τ_{i_*}), $z \in Z_{i_*-1}(z_{i_*-1}, u^{(i_*-1)}(\cdot))$.*

Definition 3. *For $0 \le i < i_* - 2$, a system state $x \in R^n$ is said to be (μ_*, Q_*) – guaranteed reachable form a position (z_i, τ_i), $z_i \in R^n$, $0 \le \tau_i$, subject to $(i_* - i)$ correction moments $\tau_{i+1}, \tau_{i+2},..., \tau_{i_*}$, if there exists a control $u^{(i)}(\cdot) \in U^{(i)}$, such that the state x is (μ_*, Q_*) – guaranteed reachable subject to $(i_* - i - 1)$ correction moments $\tau_{i+2},..., \tau_{i_*}$ from all positions (z, τ_i), $z \in Z_i(z_i, u^{(i)}(\cdot))$.*

Denote by $X_*(z_{i_*} \mid \tau_{i_*})$ the set of all system states that are (μ_*, Q_*) – guaranteed reachable (without correction) from position (z_{i_*}, τ_{i_*}). For $i = i_* - 1, ..., 0$, denote by $X_*(z_i \mid \tau_i, \tau_{i+1}, ..., \tau_{i_*})$ the set of all system states that are (μ_*, Q_*) – guaranteed reachable from position (z_i, τ_i) subject to the intermediate correction moments $\tau_{i+1}, ..., \tau_{i_*}$.

It is evident that $x \in X_*(z_i \mid \tau_i, ..., \tau_{i_*})$ if and only if there exists a control $u^{(i)}(\cdot) \in U^{(i)}$ such that $x \in X_*(z \mid \tau_{i+1}, ..., \tau_{i_*})$ for all $z \in Z_i(z_i, u^{(i)}(\cdot))$, i.e.

$X_*(z_i \mid \tau_i, ..., \tau_{i_*}) = \{x \in R^n : \exists u^{(i)}(\cdot) \in U^{(i)}$ such that $\forall\ z \in Z_i(z_i, u^{(i)}(\cdot))\}$.

The aims of the paper are the following

A. to give constructive description of the set

$$X_*(z_0 \mid \tau_0, ..., \tau_{i_*}), \tag{4}$$

i.e. to describe the set of all system state that are (μ_*, Q_*) – guaranteed reachable at the terminal moment t_* from a given initial position $(z_0, \tau_0 = 0)$ with intermediate correction moments $\tau_1, ..., \tau_{i_*}$,

B. to investigate the dependence of the set (4) on a set of correction time instances (3).

3. Different Presentations of the Reachable Set with a Fixed Set of Correction Moments

In this section, we suppose that the set of correction moments (3) is fixed. Let us describe different presentations of the reachable sets $X_*(z_i \mid \tau_i, ..., \tau_{i_*})$, $i = 0, ..., i_*$.

One can easily check that the following proposition holds true.

Proposition 1. The sets $X_*(z_i \mid \tau_i, ..., \tau_{i_*})$, $i = 0, ..., i_*$, admit the following presentations

$X_*(z_i \mid \tau_i, ..., \tau_{i_*}) = \{x \in R^n : \overline{\gamma}_i(x \mid z_i) \le \mu_*\}$,

where functions $\overline{\gamma}_i(x \mid z_i)$ $i = 0, ..., i_*$, are defined by the recursive relations

$$\overline{\gamma}_i(x \mid z_i) = \min_{u^{(i)}(\cdot) \in U^{(i)}} \max_{w^{(i)}(\cdot) \in W^{(i)}} \overline{\gamma}_{i+1}(x \mid \overline{z}_{i+1}(z_i, u^{(i)}(\cdot), w^{(i)}(\cdot))), \quad i = 0, 1, ..., i_* - 1, \tag{5}$$

with the initial condition

$$\overline{\gamma}_{i_*}(x \mid z_{i_*}) = \min_{u^{(i_*)}(\cdot) \in U^{(i_*)}} \max_{w^{(i_*)}(\cdot) \in W^{(i_*)}} \left\| \overline{z}_{i_*+1}(z_{i_*}, u^{(i_*)}(\cdot), w^{(i_*)}(\cdot)) - x \right\|^2_{Q_*}. \tag{6}$$

Here $\overline{z}_{i+1}(z_i, u^{(i)}(\cdot), w^{(i)}(\cdot)) = F(\tau_{i+1}, \tau_i) z_i + \sum_{s \in I_i} \int_{T_s} F(\tau_{i+1}, t)(b u_s(t) + g w_s(t)) dt$, $i = 0, 1, ..., i_*$, $F(t, \tau)$ is the fundament solution matrix for the system $\dot{x} = Ax$.

Remark 1. The relations (5), (6) imply that

$$\overline{\gamma}_i(x \mid z_i) = \min_{u^{(i)}(\cdot) \in U^{(i)}} \max_{w^{(i)}(\cdot) \in W^{(i)}} \min_{u^{(i+1)}(\cdot) \in U^{(i+1)}} \max_{w^{(i+1)}(\cdot) \in W^{(i+1)}} ...$$

$$... \min_{u^{(i_*)}(\cdot) \in U^{(i_*)}} \max_{w^{(i_*)}(\cdot) \in W^{(i_*)}} \| F(t_*, \tau_i) z_i + \sum_{s=m_i+1}^{N+1} \int_{T_s} F(t_*, t)(b u_s(t) + g w_s(t)) dt - x \|^2_{Q_*}.$$

Note that, in this min-max optimisation problem, decision variables are functions $u^{(s)}(\cdot), w^{(s)}(\cdot)$, $s = i, ..., i_*$.

Here and in what follows the set of indices $s = q, q+1, ..., m,$ is considered to be empty if $m < q$.

Denote

$$G_s = \int_{T_s} \big(F(t_*, t) b\big)\big(F(t_*, t) b\big)^T dt \in R^{n \times n}, \quad Q_s = \int_{T_s} \big(F(t_*, t) g\big)\big(F(t_*, t) g\big)^T dt \in R^{n \times n},$$

$$\Psi_s = \{\psi \in R^n : \psi^T G_s \psi \le r_s\}, \quad \Phi_s = \{\phi \in R^n : \phi^T Q_s \phi \le v_s\}, s = 1, ..., N+1.$$

Theorem 1. Functions (5), (6) can be presented in the form

$$\overline{\gamma}_i(x \mid z_i) = \gamma_i(x \mid F(t_*, \tau_i) z_i)\ i = 0,1,...,i_*, \tag{7}$$

where functions $\gamma_i(x \mid d),\ i = 0,...,i_*$, are determined by the following recursive relations

$$\gamma_i(x \mid d) = \min_{\psi_s \in \Psi_s, s \in I_i} \max_{\phi_s \in \Phi_s, s \in I_i} \gamma_{i+1}(x \mid d + \sum_{s \in I_i} (G_s \psi_s + Q_s \phi_s)), \quad i = 0,1,...i_* - 1, \tag{8}$$

with the initial condition

$$\gamma_{i_*}(x \mid d) = \min_{\psi_s \in \Psi_s, s \in I_{i_*}} \max_{\phi_s \in \Phi_s, s \in I_{i_*}} \| d + \sum_{s \in I_{i_*}} (G_s \psi_s + Q_s \phi_s) - x \|^2_{Q_*} . \tag{9}$$

Remark 2. The relations (8), (9) imply that

$$\gamma_i(x \mid F(t_*, \tau_i) z_i) = \min_{\psi_s, s \in I_i} \max_{\phi_s, s \in I_i} \min_{\psi_s, s \in I_{i+1}} \max_{\phi_s, s \in I_{i+1}} ... \min_{\psi_s, s \in I_{i_*}} \max_{\phi_s, s \in I_{i_*}} \| F(t_*, \tau_i) z_i + \sum_{s=m_i+1}^{N+1} (G_s \psi_s + Q_s \phi_s) - x \|^2_{Q_*}$$

subject to $\psi_s^T G_s \psi_s \le r_s,\ \phi_s^T Q_s \phi_s \le v_s,\ s = m_i + 1,..., N+1.$

Remark 3. Note that the functions $\gamma_i(x \mid d),\ i = 0,...,i_*,$ are simpler than the functions $\overline{\gamma}_i(x \mid z_i),\ i = 0,...,i_*,$ since for construction of the functions $\gamma_i(x \mid d),$ one needs to solve min-max (finite dimensional) optimisation problems with respect to the set of *n*-vectors $\psi_s, \phi_s, s \in I_k,\ k = i,...,i_*,$ while for constructing the functions $\overline{\gamma}_i(x \mid z_i),$ one has to solve min-max (infinite dimensional) optimisation problems with respect to the set of functions $u_s(\cdot), w_s(\cdot), s \in I_k,\ k = i,...,i_*.$

Proof of Theorem 1. For $i = 0,1,...,i_*$, let us consider the sets

$$Z_*(i) = \{z \in R^n : z = \sum_{s \in I_i} \int_{T_s} F(t_*, t) g w_s(t) dt,\ w_s(\cdot) \in W_s, s \in I_i\}, \tag{10}$$

$$\tilde{Z}_*(i) = \{z \in R^n : z = \sum_{s \in I_i} Q_s \phi_s,\ \phi_s^T Q_s \phi_s \le v_s, s \in I_i\}, \tag{11}$$

and show that

$$Z_*(i) = \tilde{Z}_*(i),\ i = 0,1,...,i_*. \tag{12}$$

It is evident that the sets $Z_*(i)$ and $\tilde{Z}_*(i)$ can be written in the equivalent form:

$$Z_*(i) = \{z \in R^n : z = \sum_{s \in I_i} \Delta z_s,\ \Delta z_s \in \Delta Z_s, s \in I_i\},$$

$$\tilde{Z}_*(i) = \{z \in R^n : z = \sum_{s \in I_i} \Delta \tilde{z}_s,\ \Delta \tilde{z}_s \in \Delta \tilde{Z}_s,\ s \in I_i\},$$

where $\Delta Z_s = \{\Delta z \in R^n : \Delta z = \int_{T_s} F(t_*, t) g w_s(t) dt,\ w_s(\cdot) \in W_s\},\ s = 1,..., N+1,$

$$\Delta \tilde{Z}_s = \{\Delta z \in R^n : \Delta z = Q_s \phi_s,\ \phi_s^T Q_s \phi_s \le v_s\},\ s = 1,..., N+1.$$

It follows from Lemma 1 [9, page 134] that the equalities $\Delta Z_s = \Delta \tilde{Z}_s,\ s = 1,...N+1$, take place. Evidently, these equalities imply (12).

Similarly one can show that the equalities take place

$$Z_{**}(i) = \tilde{Z}_{**}(i),\ i = 0,1,...,i_*, \tag{13}$$

with

$$Z_{**}(i) = \{z \in R^n : z = \sum_{s \in I_i} \int_{T_s} F(t_*, t) b u_s(t) dt,\ u_s(\cdot) \in U_s, s \in I_i\}, \tag{14}$$

$$\tilde{Z}_{**}(i)=\{z\in R^n : z=\sum_{s\in I_i} G_s\psi_s,\ \psi_s^T G_s\psi_s\le r_s, s\in I_i\}. \tag{15}$$

Let us prove the equality (7) for $i=i_*$, i.e. let us show that

$$\min_{u^{(i_*)}(\cdot)\in U^{(i_*)}}\max_{w^{(i_*)}(\cdot)\in W^{(i_*)}} \| F(t_*,\tau_{i_*})z_{i_*}+\sum_{s\in I_{i_*}}\int_{T_s} F(t_*,t)(bu_s(t)+gw_s(t))dt-x\|^2_{Q_*}=$$

$$=\min_{\psi_s\in\Psi_s, s\in I_{i_*}}\max_{\phi_s\in\Phi_s, s\in I_{i_*}} \| F(t_*,\tau_{i_*})z_{i_*}+\sum_{s\in I_{i_*}}(G_s\psi_s+Q_s\phi_s)-x\|^2_{Q_*}. \tag{16}$$

It is clear that

$$\min_{u^{(i_*)}(\cdot)\in U^{(i_*)}}\max_{w^{(i_*)}(\cdot)\in W^{(i_*)}} \| F(t_*,\tau_i)z_i+\sum_{s\in I_{i_*}}\int_{T_s} F(t_*,t)(bu_s(t)+gw_s(t))dt-x\|^2_{Q_*}=$$

$$=\min_{z\in Z_*(i_*)}\max_{y\in Z_{**}(i_*)} \| F(t_*,\tau_{i_*})z_{i_*}+z+y-x\|^2_{Q_*}, \tag{17}$$

$$\min_{\psi_s\in\Psi_s, s\in I_{i_*}}\max_{\phi_s\in\Phi_s, s\in I_{i_*}} \| F(t_*,\tau_{i_*})z_{i_*}+\sum_{s\in I_{i_*}}(G_s\psi_s+Q_s\phi_s)-x\|^2_{Q_*}=$$

$$=\min_{z\in\tilde{Z}_*(i_*)}\max_{y\in\tilde{Z}_{**}(i_*)} \| F(t_*,\tau_{i_*})z_{i_*}+z+y-x\|^2_{Q_*}. \tag{18}$$

Then (16) follows from (12), (13), (17), (18).

Suppose that equalities (7) are proved for $s=i+1,...,i_*$ with $i\le i_*-1$. Let us prove (7) for $s=i$. On account of (5) and (8), for this purpose, one needs to show that

$$\min_{u^{(i)}(\cdot)\in U^{(i)}}\max_{w^{(i)}(\cdot)\in W^{(i)}} \overline{\gamma}_{i+1}(x\,|\,\overline{z}_{i+1}(z_i,u^{(i)}(\cdot),w^{(i)}(\cdot)))=$$

$$=\min_{\psi_s\in\Psi_s, s\in I_i}\max_{\phi_s\in\Phi_s, s\in I_i} \gamma_{i+1}(x\,|\,F(t_*,\tau_i)z_i+\sum_{s\in I_i}(G_s\psi_s+Q_s\phi_s)), \tag{19}$$

with

$$\overline{z}_{i+1}(z_i,u^{(i)}(\cdot),w^{(i)}(\cdot))=F(\tau_{i+1},\tau_i)z_i+\sum_{s\in I_i}\int_{T_s} F(\tau_{i+1},t)(bu_s(t)+gw_s(t))dt, \tag{20}$$

It follows from (10), (14), (20) that

$$\min_{u^{(i)}(\cdot)\in U^{(i)}}\max_{w^{(i)}(\cdot)\in W^{(i)}} \overline{\gamma}_{i+1}(x\,|\,\overline{z}_{i+1}(z_i,u^{(i)}(\cdot),w^{(i)}(\cdot)))=$$

$$=\min_{z\in Z_*(i)}\max_{y\in Z_{**}(i)} \overline{\gamma}_{i+1}(x\,|\,F(\tau_{i+1},\tau_i)z_i+F^{-1}(t_*,\tau_{i+1})(z+y)).$$

and it follows from (11), (15) that

$$\min_{\psi_s\in\Psi_s, s\in I_i}\max_{\phi_s\in\Phi_s, s\in I_i} \gamma_{i+1}(x\,|\,F(t_*,\tau_i)z_i+\sum_{s\in I_i}(G_s\psi_s+Q_s\phi_s))=\min_{z\in\tilde{Z}_*(i)}\max_{y\in\tilde{Z}_{**}(i)} \gamma_{i+1}(x\,|\,F(t_*,\tau_i)z_i+z+y).$$

These equalities and equalities (12), (13), and assumption that $\overline{\gamma}_{i+1}(x\,|\,z_{i+1})=\gamma_{i+1}(x\,|\,F(t_*,\tau_{i+1})z_{i+1})$ imply relations (19), and, consequently, relations (7) for $s=i$. The theorem is proved.

Corollary 1. The sets $X_*(z_i\,|\,\tau_i,...,\tau_{i_*})$, $i=0,...,i_*,$ can be presented in the form

$$X_*(z_i\,|\,\tau_i,...,\tau_{i_*})=\{x\in R^n : \gamma_i(x\,|\,F(t_*,\tau_i)z_i)\le\mu_*\}, \tag{21}$$

where functions $\gamma_i(x\,|\,d),\ i=0,...,i_*,$ are defined according to relations (8), (9).

It follows from presentation (21) that, for given $z_i,\tau_i,\tau_{i+1},...,\tau_{i_*}$, the reachable set $X_*(z_i\,|\,\tau_i,...,\tau_{i_*})$ is the level set for the function $\gamma_i(x\,|\,F(t_*,\tau_i)z_i)$, $x\in R^n$.

Theorem 2. For $i = 0,...,i_*$, function $\gamma_i(x \mid d)$, $x \in R^n, d \in R^n$, is convex with respect to (w.r.t.) the set of variables (x,d) on $X \times D$ where X, D are some convex bounded subsets of R^n.

In proving the theorem, we will use the follow propositions.

Proposition 2. (see page 48 in [10]) Consider the function

$$f(x) = \sup_{y \in Y} \phi(x,y),\ x \in X,$$

where $X \subset R^n$ is a convex set, the function $\phi(x,y)$ is convex w.r.t. x on X for any fixed $y \in Y$, the function $f(x)$ is finite on X. Then the function $f(x)$ is convex w.r.t. to x on X.

Proposition 3. (see Lemma 4.4 in [10]) Consider the function

$$f(x) = \inf_{y \in Y} \phi(x,y),\ x \in X,$$

where $X \subset R^n$ and Y are convex sets, the function $\phi(x,y)$ is convex w.r.t. the set of variables (x,y) on $X \times Y$, the function $f(x)$ is finite on X. Then $f(x)$ is convex w.r.t. x on X.

Proposition 4. Let X, Y, Z, D be any convex bounded subsets of R^n and

$$\bar{D} = \left\{ \bar{z} \in R^n : \bar{z} = y + z + d, y \in Y, z \in Z, d \in D \right\}.$$

Suppose that the function $f(x \mid \bar{d})$ is convex w.r.t the set of variables $(x, \bar{d})$ on $X \times \bar{D}$. Then the function $\tilde{f}(x \mid y,z,d) = f(x \mid y+z+d)$ is convex w.r.t. the set of variables (x,y,z,d) on $X \times Y \times Z \times D$.

Proof of Theorem 2. It follows for the constructions presented above that the functions $\gamma_i(x \mid d)$, $i = 0,...,i_*$, can be written in the form

$$\gamma_{i_*}(x \mid d) = \min_{z \in \tilde{Z}_*(i_*)} \max_{y \in \tilde{Z}_{**}(i_*)} \| d + z + y - x \|^2_{Q_*},$$

$$\gamma_i(x \mid d) = \min_{z \in \tilde{Z}_*(i)} \max_{y \in \tilde{Z}_{**}(i)} \gamma_{i+1}(x \mid d + y + z),\ i = i_* - 1, i_* - 2, ..., 0,$$

where the sets $\tilde{Z}_*(i),\ \tilde{Z}_{**}(i),\ i = 0,...,i_*$, are defined in (11),(15) and are convex.

We will prove the theorem on the base of induction approach.

Owing to Proposition 2, the function $f_{i_*}(x,z,d) = \max_{y \in \tilde{Z}_{**}(i_*)} \| d + z + y - x \|^2_{Q_*}$ is convex w.r.t. the set of variables (x,z,d) on $X \times Z \times D$ where X, Z, D are convex subsets of R^n. Consequently, in view of Proposition 3, the function $\gamma_{i_*}(x \mid d) = \min_{z \in \tilde{Z}_*(i_*)} f_{i_*}(x,z,d)$ is convex w.r.t. the set of variables (x,d) on $X \times D$, where X, D are convex subsets of R^n.

Suppose that for some $i,\ 0 < i \le i_* - 1$, the function $\gamma_{i+1}(x \mid \bar{d})$ is convex w.r.t. the set of variables $(x, \bar{d})$ on $X \times \bar{D}$, where $X, \bar{D}$ are convex subsets of R^n. Then according to Proposition 4 function $\tilde{\gamma}_{i+1}(x,y,z,d) = \gamma_{i+1}(x \mid y+z+d)$ is convex w.r.t. the sets of variables (x,y,z,d) on $X \times Y \times Z \times D$ where X, Y, Z, D are convex subsets of R^n. Hence due to Proposition 2 the function

$$f_i(x,z,d) = \max_{y \in \tilde{Z}_{**}(i)} \tilde{\gamma}_{i+1}(x,y,z,d)$$

is convex w.r.t. the variables (x,z,d) on $X \times Z \times D$. Taking into account this fact and Proposition 3, we conclude that the function

$$\gamma_i(x \mid d) = \min_{z \in \tilde{Z}_*} f_i(x,z,d)$$

is convex w.r.t. the set of variables (x,d) on $X \times D$. The theorem is proved.

Corollary 2. For $i = 0,...,i_*$, the set $X_*(z_i \mid \tau_i,...,\tau_{i_*}) \subset R^n$ is convex (or empty).

4. Dependence of the Reachability Set on a Set of Correction Moments

Let us consider two sets of correction time instances

$\tau_1, \tau_2, ..., \tau_k, \tau_{k+1}, ..., \tau_{i_*}$ and $\tau_1, \tau_2, ..., \tau_k, \tau_*, \tau_{k+1}, ..., \tau_{i_*}$,

where $\tau_* = t_{m_*}$, $m_k < m_* < m_{k+1}$, $k \in \{0,1,...,N\}$. It follows from Theorem 1 that the sets $X_*(z_0 \mid \tau_0 = 0, ..., \tau_k, \tau_{k+1}, ..., \tau_{i_*})$ and $X_*(z_0 \mid \tau_0 = 0, ..., \tau_k, \tau_*, \tau_{k+1}, ..., \tau_{i_*})$ can be presented in the forms

$$X_*(z_0 \mid 0, \tau_1, ..., \tau_{i_*}) = \{x \in R^n : \hat{\gamma}(x \mid z_0, \tau_0, \tau_1, ..., \tau_k, \tau_{k+1}, ..., \tau_{i_*}) \le \mu_*\},$$

$$X_*(z_0 \mid 0, \tau_1, ..., \tau_k, \tau_*, \tau_{k+1}, ..., \tau_{i_*}) = \{x \in R^n : \breve{\gamma}(x \mid z_0, \tau_0, \tau_1, ..., \tau_k, \tau_*, \tau_{k+1}, ..., \tau_{i_*}) \le \mu_*\}.$$

Here

$$\hat{\gamma}(x \mid z_0, \tau_0, \tau_1, ..., \tau_k, \tau_{k+1}, ..., \tau_{i_*}) =$$

$$= \min_{\psi_s, s \in I_0} \max_{\phi_s, s \in I_0} ... \min_{\psi_s, s \in I_k} \max_{\phi_s, s \in I_k} ... \min_{\psi_s, s \in I_{i_*}} \max_{\phi_s, s \in I_{i_*}} \| F(t_*, 0) z_0 + \sum_{s=1}^{N+1} (G_s \psi_s + Q_s \phi_s) - x \|^2_{Q_*} \quad (22)$$

subject to $\psi_s^T G_s \psi_s \le r_s$, $\phi_s^T Q_s \phi_s \le v_s$, $s = 1, ..., N+1$.

The function $\breve{\gamma}(x \mid z_0, \tau_0, \tau_1, ..., \tau_k, \tau_*, \tau_{k+1}, ..., \tau_{i_*})$ is obtained from the function $\hat{\gamma}(x \mid z_0, \tau_0, \tau_1, ..., \tau_k, \tau_{k+1}, ..., \tau_{i_*})$, if in (22) operations $\min_{\psi_s, s \in I_k} \max_{\phi_s, s \in I_k}$ are replaced by $\min_{\psi_s, s \in I_k^1} \max_{\phi_s, s \in I_k^1} \min_{\psi_s, s \in I_k^2} \max_{\phi_s, s \in I_k^2}$, with $I_k^1 = \{m_k + 1, ..., m_*\}$, $I_k^2 = \{m_* + 1, ..., m_{k+1}\}$, $I_k = I_k^1 \cup I_k^2$.

Taking into account the well-known max-min inequality

$$\min_{\psi_* \in \Psi_*} \max_{\phi_* \in \Phi_*} \min_{\psi^* \in \Psi^*} \max_{\phi^* \in \Phi^*} f(\psi_*, \psi^*, \phi_*, \phi^*) \le \min_{\psi_* \in \Psi_*} \min_{\psi^* in \Psi^*} \max_{\phi_* \in \Phi_*} \max_{\phi^* \in \Phi^*} f(\psi_*, \psi^*, \phi_*, \phi^*), \quad (23)$$

we conclude that the following inclusion takes place

$$X_*(z_0 \mid 0, \tau_1, ..., \tau_k, \tau_{k+1}, ..., \tau_{i_*}) \subset X_*(z_0 \mid 0, \tau_1, ..., \tau_k, \tau_*, \tau_{k+1}, ..., \tau_{i_*}).$$

Hence we have proved the following theorem that characterizes the dependence of the reachable set on a set of correction moments.

Theorem 3. Addition of a new moment to a set of correction moments leads to the extension of the set of system states that are (μ_*, Q_*) − guaranteed reachable at the terminal moment $t = t_*$ form a fixed initial position $(z_0, 0)$.

In the next section we illustrate the theoretical result on a numerical example.

5. Numerical Experiment

Consider system (1). Suppose that $N = i_* = 1$ and the sets of moments $t_s, s = 0, ..., N+1$ and $\tau_s, s = 0, ..., i_*$, are the following

$$t_0 = 0,\ t_1 = 1,\ t_2 = 2,\ \tau_0 = t_0,\ \tau_1 = t_1. \quad (24)$$

The aim of this example is to show that the reachable set $X_*(z_0 \mid \tau_0, \tau_1)$ (with one correction moment τ_1) is wider than the reachable set $X_*(z_0 \mid \tau_0)$ (without correction moments). For the comparison of these sets, we construct the corresponding approximations. The $X_*(z_0 \mid \tau_0)$ is approximated by a set $\overline{X}_*(z_0 \mid \tau_0)$ such that $\overline{X}_*(z_0 \mid \tau_0) \supset X_*(z_0 \mid \tau_0)$ and the set $X_*(z_0 \mid \tau_0, \tau_1)$ is approximated by the set $\overline{X}_*(z_0 \mid \tau_0, \tau_1)$ such that $\overline{X}_*(z_0 \mid \tau_0, \tau_1) \subset X_*(z_0 \mid \tau_0, \tau_1)$. After that we will show that $\overline{X}_*(z_0 \mid \tau_0, \tau_1) \supset \overline{X}_*(z_0 \mid \tau_0)$ and consequently

$$X_*(z_0 \mid \tau_0, \tau_1) \supset \overline{X}_*(z_0 \mid \tau_0, \tau_1) \supset \overline{X}_*(z_0 \mid \tau_0) \supset X_*(z_0 \mid \tau_0).$$

Rules for construction of the auxiliary sets $\overline{X}_*(z_0 \mid \tau_0)$ and $\overline{X}_*(z_0 \mid \tau_0, \tau_1)$ are presented below.

5.1. Construction of the Set $\overline{X}_*(z_0 \mid \tau_0)$

For data (24), the set $X_*(z_0 \mid \tau_0)$ can be written in the form

$$X_*(z_0 \mid \tau_0) = \Big\{ x \in R^n : \min_{\psi_1} \min_{\psi_2} \max_{\phi \in \Phi_*} \| F(t_*, 0) z_0 + G_1\psi_1 + G_2\psi_2 + \phi - x \|^2_{Q_*} \le \mu_*,$$

subject to $\psi_s^T G_s \psi_s \le r_s,\ s = 1, 2\}$,

where $\Phi_* = \Big\{ y \in R^n : y = Q_1 y_1 + Q_2 y_2,\ y_s^T Q_s y_s \le v_s, s = 1, 2 \Big\}$. Consider the set

$$\overline{X}_*(z_0 \mid \tau_0) = \Big\{ x \in R^n : \min_{\psi_1} \min_{\psi_2} \max_{y \in \Phi_*^M} \| F(t_*, 0) z_0 + G_1\psi_1 + G_2\psi_2 + y - x \|^2_{Q_*} \le \mu_*,$$

subject to $\psi_s^T G_s \psi_s \le r_s,\ s = 1, 2\}$,

where Φ_*^M is a polyhedron which is external approximation for the set Φ_*. Since $\Phi_*^M \subset \Phi_*$, we have $\overline{X}_*(z_0 \mid \tau_0) \supset X_*(z_0 \mid \tau_0)$.

To construct the set $\overline{X}_*(z_0 \mid \tau_0)$ one needs to calculate the maximum of convex function over the polyhedron Φ_*^M. It is well-known that the maximum is reached at a vertex of the polyhedron Φ_*^M. Let $y_j, j \in J$, be the vertices of the polyhedron Φ_*^M. Then the set $\overline{X}_*(z_0 \mid \tau_0)$ can be written in the equivalent form: $\overline{X}_*(z_0 \mid \tau_0) = \{ x \in R^n : \xi(x) \le \mu_* \}$ where $\xi(x)$ is the optimal value of the following problem

$$\xi(x) = \min_{\xi, \psi_1, \psi_2} \xi,$$

$$\| F(t_*, 0) z_0 + G_1\psi_1 + G_2\psi_2 + y_j - x \|^2_{Q_*} \le \xi,\ j \in J,\ \ \psi_s^T G_s \psi_s \le r_s, s = 1, 2\,. \tag{25}$$

The problem (25) is a convex programming problem and its solution can be found by standard methods.

5.2. Construction of the Set $\overline{X}_*(z_0 \mid \tau_0, \tau_1)$

For data (24), the set $X_*(z_0 \mid \tau_0, \tau_1)$ can be presented in the form

$$X_*(z_0 \mid \tau_0, \tau_1) = \{ x \in R^n : \min_{\psi_1} \max_{\overline{\phi}_1 \in \Phi_*^1} \min_{\psi_2} \max_{\overline{\phi}_2 \in \Phi_*^2} \| F(t_*, 0) z_0 + G_1\psi_1 + G_2\psi_2 + \overline{\phi}_1 + \overline{\phi}_2 - x \|^2_{Q_*} \le \mu_*,$$

subject to $\psi_s^T G_s \psi_s \le r_s,\ s = 1, 2\}$,

where $\Phi_*^s = \Big\{ \overline{\phi} \in R^n : \overline{\phi} = Q_s \phi,\ \phi_s^T Q_s \phi_s \le v_s \Big\}, s = 1, 2$. Consider the set

$$\overline{X}_*(z_0 \mid \tau_0, \tau_1) = \{ x \in R^n : \min_{\psi_1} \max_{a_1 \in \Phi_*^{1M}} \min_{\psi_2} \max_{a_2 \in \Phi_*^{2M}} \| F(t_*, 0) z_0 + G_1\psi_1 + G_2\psi_2 + a_1 + a_2 - x \|^2_{Q_*} \le \mu_*,$$

subject to $\psi_s^T G_s \psi_s \le r_s,\ s = 1, 2\}$,

where Φ_*^{sM}, is a polyhedron that is an external approximation for the set Φ_*^s, $s = 1, 2$. Denote by $y_1^i, i \in J_1$, and $y_2^j,\ j \in J_2\ y_2^j, j \in J_2$, the vertices of the polyhedrons Φ_*^{1M} and Φ_*^{2M} respectively. Since $\Phi_*^{sM} \supset \Phi_*^s,\ s = 1, 2,$ then the inclusion $\overline{X}_*(z_0 \mid \tau_0, \tau_1) \subset X_*(z_0 \mid \tau_0, \tau_1)$ takes place.

Reasoning by analogy with subsection 5.1, we get the following presentation of the set $\overline{X}_*(z_0 \mid \tau_0, \tau_1)$: $\overline{X}_*(z_0 \mid \tau_0, \tau_1) = \{ x \in R^n : \xi(x) \le \mu_* \}$ where $\xi(x)$ is the optimal value of the problem

$$\xi(x) = \min_{\xi, \psi_1, \psi_{2j}, j \in J_1} \xi$$

$$\| F(t_*, 0) z_0 + G_1\psi_1 + G_2\psi_{2j} + y_1^j + y_2^i - x \|^2_{Q_*} \le \xi,\ \ j \in J_1, i \in J_2, \tag{26}$$

$$\psi_1^T G_1 \psi_1 \le r_1,\ \ \psi_{2j}^T G_2 \psi_{2j} \le r_2, j \in J_1.$$

The problem (26) is a convex programming problem. Its solution can be found by standard methods.

5.3. Example

Consider system (1) with the following initial data: $n=2,\ A=\begin{pmatrix}0 & 1\\ 0 & 0\end{pmatrix},\ b=[0,1],\ g=[1/2,3/10],$

$t_0=0,\ t_1=1,\ t_2=2,\ m_1=1,\ r_1=2,\ \ r_2=2,\ v_1=3, v_2=4,\ z_0=-[1,1],\ \mu_*=10.025,\ Q_*=\mathrm{diag}\,(1,1).$

The set Φ_* and its internal approximation Φ_*^M are shown in Figure 1.

It is easy to check that the boundary $\partial\Phi_*$ of the set Φ_* is described as follows

$$\partial\Phi_*=\{z(t)\in R: z(t)=\left(\alpha_1(t)Q_1+\alpha_2(t)Q_2\right)c(t),\ c(t)=\left(\cos(t),\sin(t)\right)^T, t\in[0,2\pi]\}$$

with $\alpha_s(t)=\sqrt{v_s/c^T(t)Q_sc(t)},\ s=1,2.$

Figures 2 and 3 show the sets Φ_*^1, Φ_*^2 and their external approximations Φ_*^{1M}, Φ_*^{2M} respectively.

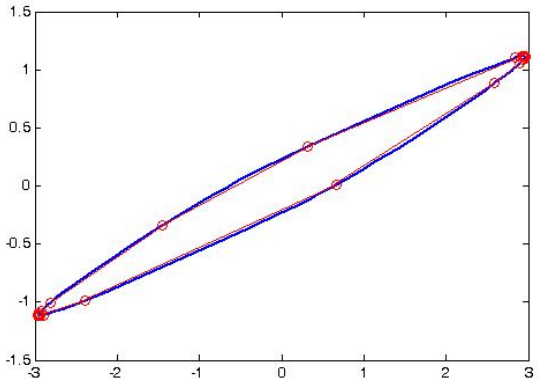

Figure 1

To construct external approximations, polyhedrons Φ_*^{1M} and Φ_*^{2M}, we choose some points $z(t_i^s), i=1,\ldots,p,$ on the boundaries

$\partial\Phi_*^{sM}=\{z(t)\in R: z(t)=\alpha_s(t)Q_sc(t),\ c(t)=\left(\cos(t),\sin(t)\right)^T, t\in[0,2\pi]\}, s=1,2,$

of the sets Φ_*^1 and Φ_*^2 respectively. For $s=1,2$ and $i=1,\ldots,p$, at a point $z(t_i^s)$ we draw the straight line that is normal to the corresponding vectors $c(t_i^s)$. Crossing points of these lines form the vertices of the polyhedrons $\Phi_*^{sM}, s=1,2.$

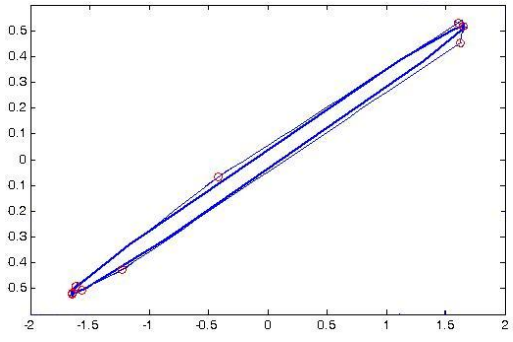

Figure 2

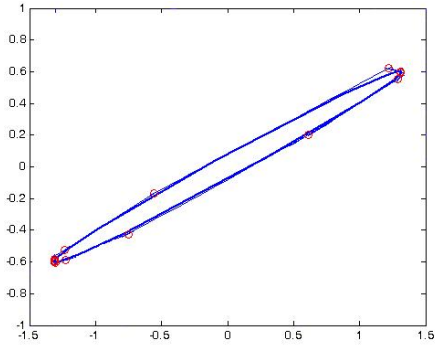

Figure 3

Figure 4 shows the sets $\overline{X}_*(z_0\mid\tau_0)$ (more dark colour) and $\overline{X}_*(z_0\mid\tau_0,\tau_1)$.

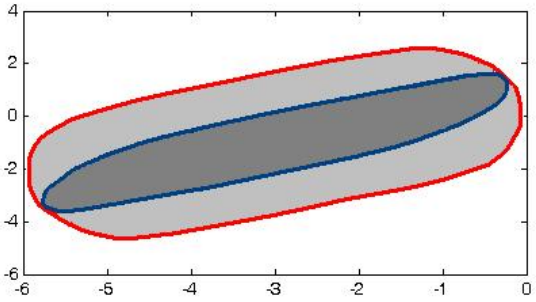

Figure 4

Since $\bar{X}_*(z_0 \mid \tau_0) \subset \bar{X}_*(z_0 \mid \tau_0, \tau_1)$, then $X_*(z_0 \mid \tau_0) \subset X_*(z_0 \mid \tau_0, \tau_1)$.

This example shows that adding one correction moment may lead to a substantial extension of the set of (μ_*, Q_*) – guaranteed reachable states of the system.

Conclusions

In the paper, we give a description of the reachable set for linear controlled system with uncertainties under assumption that control function may be corrected in some intermediate time instances.

To realize this description one needs to solve min-max optimisation problems with respect to a set of unknown functions. It is proved that these complicated optimisation problems can be reduced to simpler optimisation problems with respect to a set of unknown *n*-vectors. This allows us to give more constructive description of the reachable set.

It is proved that adding one new correction moment leads to an extension of the set of system states that are (μ_*, Q_*) – guaranteed reachable at the terminal moment t_* from a given initial position $(z_0, 0)$. Numerical example shows that this extension may be substantial. Some rules for construction external and internal approximations for the reachable sets are discussed.

References

1. Chernousko, F. *State Estimation for Dynamic Systems*. Boca Raton: CRC Press, 1994. 304 p.
2. Kurzhanski, A., Varaiya, P. Reachability under uncertainty, *SIAM Journal on Control and Optimization*, Vol. 41, No 1, 2002, pp. 181–216.
3. Kurzhanski, A. B., Varaiya, P. Reachability analysis for uncertain systems – the ellipsoidal technique, *Dynamics of Continuous, Discrete and Impulsive Systems*, Vol. 9, No 3, 2002, pp. 347–367.
4. Ovseevich, A. *Reachability domains for controlled systems, their properties, approximations and applications: Thesis for a Doctor's degree*. Moscow. 1996. 175 p.
5. Nazin, A., Nazin, S., Polyak, B. On Convergence of External Ellipsoidal Approximations of the Reachability Domains of Discrete Dynamic Linear Systems, *Automation and Remote Control*, Vol. 65, No 8, 2004, pp. 1210–1230.
6. Scokaert, P., Mayne, D. Min-max feedback model predictive control for constrained linear systems, *IEEE Transactions on Automatic Control*, Vol. 43, No 8, 1998, pp. 1136–1142.
7. Bemporad, A., Borrelli, F., Morari, M. Min-Max control of constrained uncertain discrete-time linear systems, *IEEE Transactions on Automatic Control*, Vol. 48, No 9, 2003, pp. 1600–1606.
8. Kerrigan, E., Maciejowski, J. Feedback min-max model predictive control using a single linear program: Robust stability and explicit solution, *International Journal of Robust and Nonlinear Control*, Vol. 14, 2004, pp. 395–413.
9. Kostyukova, O., Kostina, E. Robust optimal feedback for terminal linear-quadratic control problems under disturbances, *Mathematical Programming*, Vol. 107, No 1–2, 2006, pp. 131–153.
10. Demyanov, V., Vasiliev, L. *Nondifferentiable. Optimization.* Moscow: Nauka, 1981. 384 p. (In Russian)

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RANKING METHOD BASED ON THE DIFFERENCE BETWEEN WEIGHTED OUTPUT AND INPUT

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In this paper we developed a new method to establish common weights for measuring the efficiency score of Decision-Making Units (DMUs), based on multiple inputs and multiple outputs. In the new method, these common weights are estimated according to the difference between a weighted sum of outputs and a weighted sum of inputs of the DMUs. We suggest two approaches to rank the DMUs: the first method ranks the DMUs according to the absolute "net profit" (the difference between a weighted sum of outputs and a weighted sum of inputs), while the second method ranks the DMUs according to the relative efficiency score of the ratio between the a weighted sum of outputs and a weighted sum of inputs. In addition we present a method to fix objective bounds for the weights of the variables in the Data Envelopment Analysis (DEA), which is based on the above ranking method. We proved that these bounds are feasible solutions for the DEA methodology. The ranking methods are illustrated on a case study of 24 hospitals in Israel.

***Keywords**: Data Envelopment Analysis (DEA), common weights, hospitals*

1. Introduction

The purpose of the paper is to rank units (as cites, hospitals, schools, banks, etc.) according to multiple inputs and multiple outputs in the Data Envelopment Analysis (DEA) context.

The Data Envelopment Analysis (DEA) was first introduced by Charnes, Cooper and Rhodes (CCR) in 1978. The DEA is a non-parametric method to evaluate the relative efficiency of Decision-Making Units (DMU) based on multiple inputs and multiple outputs. The efficiency score is measured as a ratio between a weighted sum of outputs and a weighted sum of inputs, even if the production function is unknown. The weights are chosen so as to find the best advantage for each unit to maximize its relative efficiency, under the restriction that this score is bound by 100% efficiency. If a unit with its optimal weights receives the score efficiency of 100%, it is efficient, and for a score smaller than 100% it is inefficient. These optimal weights differ from unit to unit. There are DEA researchers that emphasize the difficulty to rank all the units on one scale, claiming that DEA provides only a dichotomy classification into two groups: efficient and inefficient. If the number of units is small relative to the number of inputs and outputs, most of the units will be efficient.

Sometimes there is a need to fix common weights to the inputs and outputs for all the units, in contrast to the DEA. The idea of Common Set of Weights (CSW) was first published by Cook, Roll and Kazakov (1989), and later tested and reformulated by Roll, Cook and Golany (1991). There are several aims for the use of these common weights; the first one boils down to the fact that for the normalized data, the common weights indicate the importance of each factor (input/output) to determine the efficiency of the units. One can utilize these common weights to disregard factors (inputs/outputs) with very small importance. The idea of the importance of the factors has been discussed by Sengupta (1990), Arnold et al. (1996). Especially in the cases when weights are negative, one can examine if this factor was chosen in the right set, namely if it is output (input) instead of input (output). The second aim of common weights is to help us to define the bounds for the weights of inputs/outputs for the DEA method. The common weights may be the mid point of the range of the bounds of each weight. The third aim is to rank all the units with the common weights on one scale and not as in DEA where weights vary from unit to unit.

There are several methods in the literature for establishing the common weights while each method implements another objective function for this purpose. We shell present a few methods:

1) The Canonical Correlation Analysis (CCA) method, {Friedman and Sinuany-Stern (1997)}. In this method, the objective function for finding the common weights for the inputs and outputs is to maximize the correlation between a weighted sum of outputs and a weighted sum of inputs.

2) The Discriminant Analysis of Ratio (DR/DEA) method, {Sinuany-Stern and Friedman (1998)}. In this method, the discrimination into two groups: efficient and inefficient sets from the DEA, is first carried out. The objective function in this method is to maximize the discrimination between the means of these two groups.

3) The Global Efficiency (GE) method, {Ganley and Cubbin (1992)}; this method focuses on the measurement of aggregate technical efficiency by using common weights for all units. The objective function is to maximize the sum of the efficiency scores of all the units, where each efficiency score is the ratio between a weighted sum of outputs and a weighted sum of inputs. This is done by obtaining the optimal solution by one programming. It can be well-recognized that the latter comes in contrast to the DEA which advocates the solution of the linear programming *n* times, generating a separate set of optimal weight for each unit. The disadvantage of the GE method boils down to the fact that its objective function is nonlinear; therefore the solution is not obviously optimal. Some more methods for determining common weights are given in the literature review of Adler et al. (2002).

The purpose of our paper is to develop a new ranking method designated as SDEA that is based on multiple inputs and multiple outputs, with common weights for all units. Our method focuses on the difference between a weighted sum of outputs and a weighted sum of inputs, namely the "net profit". The objective function of this method is to maximize the sum of the "net profits" of all the units. The idea of maximizing the difference between the weighted outputs to the weighted inputs, for each unit, with weights that vary from unit to unit has been suggested in the past as the Additive model {see Charnes et al. (1985)}, and some of its ideas were further developed by Ali and Lerme (1997).

In addition we present a method to fix objective bounds for the weights of the variables in the DEA, which is based on the above ranking method. We proved that these bounds are feasible solutions for the DEA methodology. The ranking methods are illustrated on a case study of 24 hospitals in Israel, in order to single out the most efficient one. We choose 2 inputs: the number of standardized beds in the end of 2003, the number of standardized beds in day care (ambulatory), as well as 3 outputs: the number of total discharges in 2003, the number of hospitalisation days during 2003 and the same in ambulatory care.

Our paper is presented as follows: Section 2 introduces the SDEA method; a numerical example is outlined in Section 3. Section 4 contains the summary and conclusions.

2. Essentials of SDEA

Our new ranking method finds the common set of weights of the inputs/outputs where the objective function is to maximize the sum of all the "net profits" of the DMUs under two types of constraints. The first one is that for each DMU, its net profit can't be positive as the DEA methodology and the Global Efficiency (GE) method (see *Appendix*). The second one is that the common weights are bonded from below by some value ε suggested by Sueyoshi (1999).

Consider n Decision-Making Units (DMUs), when each DMU j $(j=1,...,n)$ utilizes m inputs $X_j=\left(X_{1j},X_{2j},.....,X_{mj}\right)^T>0$ for producing s outputs $Y_j=\left(Y_{1j},Y_{2j},.....,Y_{sj}\right)^T>0$. In this case, $\sum_{r=1}^{s} U_r Y_{rj}$ represents the weighted sum of outputs of DMU j, $\sum_{i=1}^{m} V_i X_{ij}$ stands for the weighted sum of inputs of DMUj. The net profit of DMUj may be therefore calculated as $S_j=\sum_{r=1}^{s} U_r Y_{rj}-\sum_{i=1}^{m} V_i X_{ij}$.

The objective function is: $Z=\max \sum_{j=1}^{n}\left(\sum_{r=1}^{s} U_r Y_{rj}-\sum_{i=1}^{m} V_i X_{ij}\right)=\max \sum_{j=1}^{n} S_j$. The constraints are: the net profit is less or equal to zero, namely $S_j=\sum_{r=1}^{s} U_r Y_{rj}-\sum_{i=1}^{m} V_i X_{ij}\le 0$.

We obtain thus the linear problem

$$Z = \max \sum_{j=1}^{n} \left(\sum_{r=1}^{s} U_r Y_{rj} - \sum_{i=1}^{m} V_i X_{ij} \right) = \max \sum_{j=1}^{n} S_j$$

s.t.

$$S_j = \sum_{r=1}^{s} U_r Y_{rj} - \sum_{i=1}^{m} V_i X_{ij} \le 0 \quad j=1,2,..,n \tag{1}$$

$$U_r \ge \varepsilon_r^+ > 0 \quad r=1,2,..,s$$

$$V_i \ge \varepsilon_i^- > 0 \quad i=1,2,..,m$$

Our method differs from GE in two characteristics: first, our method can be solved by means of linear programming so that the optimal solution may be obtained, and second, our method bases on the difference between the weighted sum of outputs and weighted sum of inputs and not on the ratio between the weighted sum of outputs and the weighted sum of inputs.

The Dual Problem

Let us define a dual variable λ_j that is fitted to the constraint of each unit j and the dual variables L_r^+ and L_i^- that are fitted to the constraints of each output/input, respectively. The dual problem will be defined as follows:

$$V = \min \left\{ \sum_{r=1}^{s} \varepsilon_r^+ L_r^+ + \sum_{i=1}^{m} \varepsilon_i^- L_i^- \right\}$$

s.t.

$$\sum_{j=1}^{n} \lambda_j Y_{rj} + L_r^+ \ge \sum_{j=1}^{n} Y_{rj} \quad r=1,2,..,s$$

$$-\sum_{j=1}^{n} \lambda_j X_{ij} + L_i^- \ge -\sum_{j=1}^{n} X_{ij} \quad i=1,2,..,m \tag{2}$$

$$\lambda_j \ge 0 \quad j=1,2,..,n$$

$$L_r^+ \le 0 \quad r=1,2,..,s$$

$$L_i^- \le 0 \quad i=1,2,..,m$$

Lemma 1

$$\underline{\text{If}} \quad S_j^* = \sum_{r=1}^{s} U_r^* Y_{rj} - \sum_{i=1}^{m} V_i^* X_{ij} = 0 \ \ \forall j=1,2,..,n \ \ \underline{\text{then}} \ \ \frac{1}{n} \sum_{j=1}^{n} \lambda_j^* = 1 .$$

Proof: If $S_j^* = \sum_{r=1}^{s} U_r^* Y_{rj} - \sum_{i=1}^{m} V_i^* X_{ij} = 0 \ \ \forall j=1,2,..,n$ then $Z^* = 0$.

According to the strong duality property [23] there exist $Z^* = V^* = 0$ therefore $\text{Min} \left\{ \sum_{r=1}^{s} \varepsilon_r^+ L_r^+ + \sum_{i=1}^{m} \varepsilon_i^- L_i^- \right\} = 0$ and because $\varepsilon_r^+ > 0$ $r=1,2,..,s$ $\varepsilon_i^- > 0$ $i=1,2,..,m$ and

$L_r^+ \le 0$ r=1,2,..,s $L_i^- \le 0$ i=1,2,..,m then $L_r^+ = 0 \ \forall$r=1,2,..,s $L_i^- = 0 \ \forall$i=1,2,..,m. In addition all the variables of the primal problem exist in the basis, therefore according to the complementary slackness theory $\sum_{j=1}^{n} \lambda_j^* Y_{rj} = \sum_{j=1}^{n} Y_{rj}$ r=1,2,..,s. This constraint can be written as:

$\sum_{j=1}^{n} (\lambda_j^* - 1) Y_{rj} = 0$ r=1,2,..,s the same for the constraints on the inputs. The solution of these constraints gives the following solution $\lambda_j^* = 1 \ \ \forall j = 1, 2, .., n$, therefore $\frac{1}{n} \sum_{j=1}^{n} \lambda_j^* = 1$. ■

Ranking according to SDEA

We suggest two methods to rank the DMUs, the first method ranking the DMUs according to the absolute "net profit" (the difference between a weighted sum of outputs and a weighted sum of inputs), and the second method ranking the DMUs according to the relative efficiency score of the ratio between the weighted sum of outputs and the weighted sum of inputs.

Let us define the "net profit" S_j^* of DMU j as: $S_j^* = \sum_{r=1}^{s} U_r^* Y_{r_j} - \sum_{i=1}^{m} V_i^* X_{i_j}$,

where:

U_r^* and V_i^* are the optimal common weights from the SDEA method, and they are the same for the two ranking approaches;

if S_j=0 the DMU j is efficient;

if S_j<0 the DMU j is inefficient.

The first method to rank the DMUs

The ranking is based on the "net profit" of each unit. The score is determined as $S_j^* = \sum_{r=1}^{s} U_r^* Y_{r_j} - \sum_{i=1}^{m} V_i^* X_{i_j}$. The DMU that received the highest S_j^* is ranked in the first place.

In this method the ranking is dependent on the size of the DMU's.

The second method to rank the DMUs

In this case, the DMUs are ranked according to the relative efficiency score of the ratio between the weighted sum of outputs and a weighted sum of inputs. The ranking score is determined by:

$$T_k = 1 + \frac{S_k^*}{\sum_{i=1}^{m} V_i^* X_{ik}} = \frac{\sum_{i=1}^{m} V_i^* X_{ik} + \sum_{i=1}^{m} U_r^* Y_{rk} - \sum_{i=1}^{m} V_i^* X_{ik}}{\sum_{i=1}^{m} V_i^* X_{ik}} = \frac{\sum_{i=1}^{m} U_r^* Y_{rk}}{\sum_{i=1}^{m} V_i^* X_{ik}} .$$

Bounded weights in SDEA

In order to prevent the trivial solution where all weights are zero in the SDEA method $U_r = 0 \ \forall$r=1,2,..,S and $V_i = 0 \ \forall$i=1,2,..,m and therefore $S_j = 0 \ \ \forall$j=1,2,..,n, it is necessary to set a lower bound to the weights.

This issue has been extensively dealt with in scientific literature.

The first research on bounds on the weights by a "Non Archimedean Quantity" (NAQ) was carried out by Charnes et al. (1979, 1984). Thompson et al. (1990) established the so-called assurance region (AR) in order to outline a region for the possible values of the weights. The information on the assurance region originates from experts' opinions, common sense, or previous experience.

Sueyoshi (1999) suggested restricting the weights only by a lower bound which will be a function of the number of inputs and outputs. In the literature there are many papers on methods for determining the bounds on the weights: Cooper et al. (1999), Thompson et al. (1995), Roll et al. (1991), Dyson et al. (1988). The main purpose of the constraints on the weights is to reduce the number of efficient units and also to avoid the problems of extreme values of the weights.

In our research, we adopt the Sueyoshi approach. It can be well-recognized that the primary and dual problems in the SDEA method will appear therefore as:

Primary problem

$$Z = \max \sum_{j=1}^{n} \left(\sum_{r=1}^{s} U_r Y_{rj} - \sum_{i=1}^{m} V_i X_{ij} \right) = \max \sum_{j=1}^{n} S_j$$

s.t.

$$S_j = \sum_{r=1}^{s} U_r Y_{rj} - \sum_{i=1}^{m} V_i X_{ij} \le 0 \quad j=1,2,..,n \qquad (3)$$

$$U_r \ge \frac{1}{(m+S)\max\limits_{j}\{Y_{rj}\}} \quad r=1,2,..,s$$

$$V_i \ge \frac{1}{(m+S)\max\limits_{j}\{X_{ij}\}} \quad i=1,2,..,m$$

Dual problem

$$V = \min\left\{ \sum_{r=1}^{s} \frac{1}{(m+S)\max\limits_{j}\{Y_{rj}\}} L_r^{+} + \sum_{i=1}^{m} \frac{1}{(m+S)\max\limits_{j}\{X_{ij}\}} L_i^{-} \right\}$$

s.t.

$$\sum_{j=1}^{n} \lambda_j Y_{rj} + L_r^{+} \ge \sum_{j=1}^{n} Y_{rj} \quad r=1,2,..,s \qquad (4)$$

$$-\sum_{j=1}^{n} \lambda_j X_{ij} + L_i^{-} \ge -\sum_{j=1}^{n} X_{ij} \quad i=1,2,..,m$$

$$\lambda_j \ge 0 \quad j=1,2,..,n$$

$$L_r^{+} \le 0 \quad r=1,2,..,s$$

$$L_i^{-} \le 0 \quad i=1,2,..,m$$

Lower bound on weights in SDEA

The constraint that normalizes the weighted sum of inputs $\left(\sum_{i=1}^{m} V_i^k X_{ik} = 1 \right)$ in the classical DEA approach may result in difficulties to attain a feasible solution, or, in certain cases, in creating non-realistic solutions. We suggest a new method for implementing bounds on the weights in the DEA.

The procedure that is capable of preventing the above mentioned difficulties may be presented in the following steps:

Step 1. Solve the optimization problem of SDEA of Eq. (1) and find out from it the common weights of all the inputs and outputs, V_i $i = 1,2,..,m$ $U_r = 1,2,..,s$.

Step 2. Calculate the maximal value over all the n units, of the weighted inputs from the SDEA model in *Step 1*, namely $UL = \max\limits_{j}\left\{ \sum_{i=1}^{m} V_i X_{ij} \right\}$.

Step 3. Calculate the ratio of the common weights V_i and U_r to the maximal value *UL* calculated in *Step 2*, that is $\frac{V_i}{UL}$ $i = 1,2,..,m$ and $\frac{U_r}{UL}$ $r = 1,2,..,s$. These are the fitted bounds for the weights that will solve all the problems and will give a suitable solution.

Lemma 2

The efficiency score based on common weights (SDEA method) is always less than the efficiency score in the DEA.

Proof: The DEA score is the maximal score that a unit can receive. If we restrict the problem to find only common weights, these weights produce a score smaller than the one with the varying weights, as defined in DEA methodology. ■

Lemma 3

Let us denote $UL = \max_j \left(\sum_{i=1}^{m} V_{i(CW)} X_{ij} \right)$ then $V_i(DEA) \geq \varepsilon_i^- = \frac{V_i(CW)}{UL}$ i = 1,2,.., m and $U_r(DEA) \geq \varepsilon_r^+ = \frac{U_r(CW)}{UL}$ r = 1,2,.., s , are a feasible solution for unit j by the DEA model.

Proof:

$$(1)\ S_j = \sum_{r=1}^{s} U_{r(CW)} Y_{rj} - \sum_{i=1}^{m} V_{i(CW)} X_{ij} \leq 0 \quad \forall j = 1,2,..,n \Rightarrow E_j = \frac{\sum_{r=1}^{s} U_{r(CW)} Y_{rj}}{\sum_{i=1}^{m} V_{i(CW)} X_{ij}} \leq 1 \quad \forall j = 1,2,..,n$$

$$(2)\ \mathrm{UL} = \max_j \left\{ \sum_{i=1}^{m} V_{i(CW)} X_{ij} \right\}$$

$$\text{from (2)}: \ (3)\ \frac{\sum_{i=1}^{m} V_{i(CW)} X_{ij}}{\mathrm{UL}} \leq 1 \quad \forall\ j = 1,2,..,n$$

$$\text{from (1) and (3)}: (4)\ \frac{\sum_{r=1}^{s} U_{r(CW)} Y_{rj}}{UL} \leq \frac{\sum_{i=1}^{m} V_{i(CW)} x_{ij}}{\mathrm{UL}} \leq 1 \Rightarrow \frac{\sum_{r=1}^{s} U_{r(CW)} Y_{rj}}{UL} \leq 1$$

$$(5)\ \sum_{i=1}^{m} V_{i(DEA)} X_{ij} = 1 \Rightarrow \sum_{i=1}^{m} V_{i(DEA)} X_{ij} \geq \frac{\sum_{i=1}^{m} V_{i(CW)} X_{ij}}{UL}$$

$$(6)\ \sum_{r=1}^{s} U_{r(DEA)} Y_{rj} \leq 1$$

Therefore the solutions that were defined by the above bounds $U_r(DEA) \geq \frac{U_r(CW)}{UL}$ r = 1,2,.., s , represent a feasible solution for the DEA model. ■

3. The Case Study on Israeli Hospitals

Hospitals account for about 40% of Israel's national health expenditure in 2003. This is the largest category of spending on health; community clinics, including those providing preventive medicine, account for about 38% of this expenditure [Central Bureau of Statistics (CBS) 2003].

3.1. Output and Input Measures

The main problem that appears in hospitals research concerning the DEA is that there are many types of inputs and outputs. The choice of the inputs/outputs influences the results of the efficiency of the hospitals. Therefore a literature review on DEA efficiency of hospitals was done in our research. A total of 42 publications on the regarded issue was studied, out of which we shall outline the most important

and relevant to the discussed subject: O'Neill (1988), reported on the efficiency of 27 hospitals in USA. Al-Shammari (1999) reported on the efficiency of 15 government hospitals in Jordan. Hofmarcher et al. (2002) reported on the efficiency of 15 hospitals in Austria. Kirigia et al. (2002) reported on the efficiency of 54 government hospitals in Kenya, Gruca and Nath (2000) reported on the efficiency of 168 hospitals in Canada. Grosskof et al. (2001) reported on the efficiency of 236 teaching hospitals and 556 non-teaching hospitals. Hao and Pegels (1994) reported on the efficiency of 93 medical centres.

The data reported in the references summarize the main inputs and outputs measures used in different DEA hospital studies. Evidently the most used input is no. of beds (52% of studies). Cost is used in 48% of the studies, supplies in 44% and employees in 41% of the studies.

Due to the lack of data on these additional inputs we did not include them in our study. However they all are reported in the literature as related to the number of beds, since the budget is largely derived by number of beds.

From the database available to us from the Health Ministry we used 2 inputs and 3 outputs. The inputs are: the number of standardized beds in the end of 2003 (X_1), the number of standard beds in day care (ambulatory) (X_2). The outputs are: the number of total discharges in 2003 (Y_1), the number of hospitalisation days during 2003 (Y_2) and the same in ambulatory care (Y_3).

Day care (ambulatory) has been a venue for increasing the efficiency of hospitals in Israel. Thus, we included it in our input and output variables. Overall the input/output variables we have used are those common in the literature.

The list of hospitals in Israel includes 45 hospitals. We deleted hospitals that did not have internal care and outpatient clinics (day care) units. Consequently, 24 hospitals were left for our study. The data is presented in *Table 1*, which includes information on the 24 hospitals with 3 outputs and 2 inputs.

Table 1. The numerical data

No.	DMU	INPUT		OUTPUT		
		X_1	X_2	Y_1	Y_2	Y_3
1	Asaf Harofe – Zrifin	675	72	53,017	220,017	16,535
2	Asuta – Tel Aviv	148	12	24,127	35,748	905
3	Bikur Holim – Jerusalem	193	8	16,116	62,865	465
4	Bney Zion – Haifa	366	16	32,411	124,478	1,483
5	Barzilai – Ashkelon	448	40	33,577	145,554	9,433
6	E.M.M.S – Nazaret	108	4	11,056	37,252	1,398
7	Emek – Afula	415	38	33,492	131,009	5,753
8	Hadassa (Ein Karem) – Jerusalem	618	70	49,631	226,015	23,849
9	Hadassa (Har Hatzofim) – Jerusalem	215	23	24,239	85,459	7,265
10	Hagalil Hamaaravi – Naharia	499	17	54,379	225,010	2,765
11	Hilel Yafe – Hadera	394	14	32,234	129,435	1,393
12	Kaplan – Rehovot	535	75	51,688	189,197	9,403
13	Lady Davis – Haifa	403	23	32,030	153,140	6,435
14	Laniado – Natania	207	32	24,631	96,605	5,069
15	Meir – Kfar Saba	639	55	56,016	213,304	7,416
16	Rabin (Belinson) – Petah Tikva	949	71	71,766	304,311	28,735
17	Rabin (Golda) – Petah Tikva	321	15	32,358	110,128	1,193
18	Rambam – Haifa	858	40	68,113	287,528	48,391
19	Rivka Ziv – Tzfat	315	10	22,136	91,151	3,763
20	Shearay Tsedek – Jerusalem	378	26	31,661	155,705	2,726
21	Shiba – Tel Hashomer, Ramat Gan	984	100	72,187	323,055	18,932
22	Soraski – Tel Aviv, Jaffa	984	76	82,527	354,925	21,532
23	Soroka – Beer Sheva	911	46	75,698	306,468	24,056
24	Wollfson – Holon	618	30	58,338	230,186	9,647

Table 2. The scores and the ranking of the DMUs

DMU	METHOD 1		METHOD 2	
	SCORE	RANK	SCORE	RANK
Asaf Harofe – Zrifin	-0.1759	22	0.6983	20
Asuta – Tel Aviv	0.0000	2	1.0000	2
Bikur Holim – Jerusalem	-0.0390	7	0.7247	17
Bney Zion – Haifa	-0.0627	10	0.7680	13
Barzilai – Ashkelon	-0.1142	17	0.6925	22
E.M.M.S – Nazaret	-0.0069	4	0.9123	5
Emek – Afula	-0.1128	16	0.6740	23
Hadassa (Ein Karem) – Jerusalem	-0.1145	18	0.7887	11
Hadassa (Har Hatzofim) – Jerusalem	-0.0098	5	0.9475	4
Hagalil Hamaaravi – Naharia	0.0000	2	1.0000	2
Hilel Yafe – Hadera	-0.0751	14	0.7360	16
Kaplan – Rehovot	-0.1436	19	0.7117	19
Lady Davis – Haifa	-0.0650	11	0.7890	10
Laniado – Natania	-0.0236	6	0.8814	6
Meir – Kfar Saba	-0.1482	20	0.7181	18
Rabin (Belinson) – Petah Tikva	-0.1781	23	0.7655	14
Rabin (Golda) – Petah Tikva	-0.0412	8	0.8275	9
Rambam – Haifa	0.0000	2	1.0000	2
Rivka Ziv – Tzfat	-0.0683	12	0.6963	21
Shearay Tsedek – Jerusalem	-0.0701	13	0.7649	15
Shiba – Tel Hashomer, Ramat Gan	-0.2868	24	0.6587	24
Soraski – Tel Aviv, Jaffa	-0.1684	21	0.7875	12
Soroka – Beer Sheva	-0.1059	15	0.8453	8
Wollfson – Holon	-0.0563	9	0.8782	7

Table 3. Common weights values

	FOR NORMAL VALUES	FOR REGULAR VALUES
U1	0.327141	0.00065074
U2	0.207787	0.002
U3	0.2	3.964E-06
V1	0.640326	5.8544E-07
V2	0.2	4.133E-06

It turns out that $\max_j \left\{ V_i X_{ij} \right\} = 0.8403$ and the bounds in the DEA method may be estimated therefore as listed in *Table 4*:

Table 4. Bounds in the DEA method

	FOR NORMAL VALUES	FOR REGULAR VALUES
U1	0.00065074	0.000774387
U2	0.002	0.002380028
U3	3.964E-06	4.71727E-06
V1	5.8544E-07	6.9668E-07
V2	4.133E-06	4.91833E-06

Summary and Conclusions

The following main conclusions can be drawn from the study:

In this paper we developed a new method to establish common weights for measuring the efficiency score of DMUs, based on multiple inputs and multiple outputs. In the new method, these common weights are estimated according to the difference between a weighted sum of outputs and a weighted sum of inputs of the DMUs. We suggest two approaches to rank the DMUs: the first method ranks the DMUs according to the absolute "net profit" (the difference between a weighted sum of outputs and a weighted sum of inputs), while the second method ranks the DMUs according to the relative efficiency score of the ratio between the a weighted sum of outputs and a weighted sum of inputs. If the DMUs have similar size of inputs and outputs, the ranking is similar. If not, the ranking is different. Which method is better? There is no ultimate answer, it depends on the context.

We have proved that weights obtained by the suggested procedure when divided by the weighted sum of inputs, can effectively serve as a lower bound for the DEA method. We have implemented this procedure for quality ranking of 24 hospitals in Israel. It appears that 3 hospitals (Asuta – Tel Aviv, Hagalil Hamaaravi – Naharia and Rambam – Haifa) out of the total amount proved to be efficient (their score was equal to 1), while the rest occupied positions 4–24. The ranking of the efficient hospitals proves to be the same for both suggested DEA approaches, while the inefficient ones tended to display significant differences for both types of ranking. One may appreciate the importance of the weights for normalized values of the scores as well.

Should we sub-divide the total amount of hospitals into 3 groups according to their accommodating capacity (small ones – up to 420 beds, intermediate – from 420 to 700 beds, and the big ones – more than 700 beds), it can be well-recognized that small hospitals mostly tend to obtain higher scores by the first type of ranking, while the big ones, on the contrary, are ranked higher by the second DEA approach (e.g., the Bikur Holim – Jerusalem hospital, which is a small one, was ranked the 7^{th} by the first procedure and the17^{th} by the second one, while the Rabin-Petach Tikva hospital, which is a big one – the 23^{rd} and the14^{th}, respectively, and the same for Soraski – Tel-Aviv hospital – the 21^{st} and the 12^{th}).

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References

1. Adler, N., Friedman, L., Sinuany-Stern, Z. Review of ranking methods in the DEA context, *European Journal of Operational Research*, Vol. 140, 2002, pp. 249–265.
2. Al-Ahammari, M. A multi-criteria DEA model for measuring the productive efficiency of hospitals, *Intimation journal of Operations and Production Management*, Vol. 19, 1999, pp. 879–890.
3. Ali, A. I., Lerme, S. C. Comparative advantage and disadvantage in DEA, *Annals of Operations Research*, Vol. 73, 1997, pp. 215–232.
4. Arnold, V., Bardhan, I. R., Copper, W. W., Kumbhakar, S. C. New uses of DEA and statistical regressions for efficiency evaluation and estimation-with an illustrative application to public secondary schools in Texas, *Annals of Operations Research*, Vol. 66, 1996, pp. 255–278.
5. Burgess, J. F. Jr., Wilson, P. W. Variation in efficiency among US hospitals, *INFOR*, Vol. 36, 1998, pp. 84–102.
6. Charnes, A., Cooper, W. W., Golany, B., Seiford, L., Stutz, J. Foundations of Data Envelopment Analysis for Pareto-Koopmans efficient empirical production functions, *Journal of Econometrics*, Vol. 30, 1985, pp. 91–107.
7. Charnes, A., Cooper, W. W. The Non-Archimedean CCR ratio for efficiency analysis: A rejoinder to Boyyd and Fare, *European Journal of Operational Research*, Vol. 15, 1984, pp. 333–334.
8. Charnes, A., Cooper, W. W., Rhodes, E. Short Communication: Measuring the efficiency of decision making units, *European Journal of Operational Research*, Vol. 3, 1979, p. 339.
9. Charnes, A., Cooper, W. W., Rhodes, E. Measuring the efficiency of decision making units, *European Journal of Operational Research*, Vol. 2, 1978, pp. 429–444.
10. Chernichovsky, D., Chinitz, D. The political economy of health system reform in Israel, *Health Economics*, Vol. 4, 1995, pp. 127–141.

11. Chernichovsky, D. Health system reforms in industrialized democracies: An emerging paradigm, *The Milbank Quarterly*, Vol. 73**,** No 3, 1995, pp. 339–372.
12. Cook, W. D., Roll, Y., Kazakov, A. A Data Envelopment Analysis model for measuring the relative efficiency of highway maintenance patrols, *INFOR*, Vol. 28, No 2, 1989, pp. 113–124.
13. Cooper, W. W., Kyung, S., Gang, Yu. IDEA and AR-IDEA: Models for dealing with imprecise data in DEA, *Management Science*, Vol. 45, No 4, 1999, pp. 597–607.
14. Cooper, W. W., Tone, K. Measures of inefficiency in DEA and sto-chastic frontier estimation, *European Journal of Operational Research*, Vol. 99, 1997, pp. 72–88.
15. Dyson, R. G., Thanassoulis, E. Reducing weight flexibility in data envelopment analysis, *Journal of Operational Research Society*, Vol. 39, 1988, pp. 563–576.
16. Friedman, L., Sinuany-Stern, Z. Scaling units via the canonical correlation analysis in the DEA context, *European Journal of Operational Research*, Vol. 100, No 3, 1997, pp. 629–637.
17. Ganely, J. A., Cubbin, S. A. *Public Sector Efficiency Measurement: Applications of Data Envelopment Analysis*. North-Holland, 1992.
18. Grosskopf S., Margaritis, D., Valdmanis, V. Comparing teaching and non-teaching hospitals: A frontier approach, *Health Care Management Science*, Vol. 4, 2001, pp. 83–90.
19. Grucha, T. S., Nath, D. The technical efficiency of hospitals under a single payer system: The case of Ontario community hospitals, *Health Care Management Science*, Vol. 4, 2001, pp. 91–101.
20. Gur, O., Grau, I. Hospital trust – The missing link in the Israeli health system reform, *Rive'on Lekalkala*, 1997, pp. 721–754. (In Hebrew)
21. Hao, S., Pegels, C. C. Evaluation relative efficiency of veterans affairs medical centers using DEA, *Journal of Medical Systems*, Vol. 18, No 2, 1994, pp. 55–67.
22. *Health in Israel 2001 Selected Data*. State of Israel, Ministry of Health, 2001. (In Hebrew)
23. Hillier, F. S., Lieberman, G. J. *Introduction to Operations Research, 6th ed*. McGraw-Hill, Inc., 1995.
24. Hofmarcher, M. M., Paterson, L., Riedel, M. Measuring hospital efficiency in Austria – A DEA approach, *Health Care Management Science*, Vol. 5, 2002, pp. 7–14.
25. Hollingsworth, B., Dawson, P. J., Maniadakis, N. Efficiency measurement of health care: A review of non-parametric methods and applications, *Health Care Management Science*, Vol. 2, 1999, pp. 161–172.
26. Jacobs, R. Alternative methods to examine hospital efficiency: Data Envelopment Analysis and Stochastic Frontier Analysis, *Health Care Management Science*, Vol. 4, 2001, pp. 103–115.
27. Kirigia, J. M., Emrouznejad, A., Sambo, G. L. Measurement of technical efficiency of public hospitals in Kenya: using DEA, *Journal of Medical Systems*, Vol. 26, No 1, 2002, pp. 39–45.
28. Maniadakis, N, Hollingsworth, B., Thanassoulis, E. The impact of the internal market on hospital efficiency, productivity and service quality, *Health Care Management Science*, Vol. 2, 1999, pp. 75–85.
29. Morey, R. C., Retzlaff-Roberts, D. L., Fine, D. L. Getting something for nothing: Estimating service level improvements possible in hospitals, *International Transactions in Operational Research*, Vol. 1, No 3, 1994, pp. 285–292.
30. Nunamaker, T. R. Measuring routine nursing service efficiency: A comparison of cost per patient day and data envelopment analysis models, *Health Serv. Res.* , Vol. 18, 1983, pp. 183–205.
31. O'Neill, L. Multifactor efficiency in DEA with an application to urban hospitals, *Health Care Management Science*, Vol. 1, 1998, pp. 19–27.
32. Olesen, O. B., Petersen, N. C. The use of Data Envelopment Analysis with probabilistic assurance regions for measuring hospital efficiency, *Journal of Productivity Analysis*, Vol. 17, 2002, pp. 83–109.
33. Prior, D., Sola, M. Technical efficiency and economies of diversification in health care, *Health Care Management Science*, Vol. 3, 2000, pp. 299–307.
34. Roll, Y., Cook, W. D., Golany, B. Controlling factor weights in data envelopment analysis, *IIE Transactions*, Vol. 23, 1991, pp. 2–9.
35. Sengupta, J. K. Tests of efficiency in data envelopment analysis, *Computers Operation Research*, Vol. 17, No 2, 1990, pp. 123–132.
36. Sinuany-Stern, Z., Friedman, L. Rank units using the DEA and the discriminant analysis of ratios for ranking units, *European Journal of Operational Research*, Vol. 111, No 3, 1998, pp. 470–478.
37. Sommersguter-Reiehmann, M. The impact of the Austrian hospital financing reform on hospital productivity: Empirical evidence on efficiency and technology changes using a non-parametric input-based Malmquist approach, *Health Care Management Science*, Vol. 3, 2000, pp. 309–321.

38. Stigler, G. J. The theory of economic regulation, *The Bell Journal of Economics and Management Science*, Vol. 2, No 1, 1971, pp. 3–21.
39. Sueyoshi, T. DEA non-parametric ranking test and index measurement: Slack-adjusted DEA and an application to Japanese agriculture cooperatives, *Omega*, Vol. 27, 1999, pp. 315–326.
40. Thompson, R. G., Dharmapala, P. S., Thrall, R. M. Linked cone DEA profit ratios and technical efficiency with application to Illinois coal mines, *International Journal of Production Economics*, Vol. 39, 1995, pp. 99–115.
41. Thompson, R. G., Langemeier, L. N., Lee, C.-T., Lee, E., Thrall, R. M. The role of multiplier bounds in efficiency analysis with application to Kansas farming, *Journal of Econometrics*, Vol. 46, No 2, 1990, pp. 93–108.

Appendix

The Global Efficiency Method (GE)

The global efficiency (GE) focuses on the measurement of aggregate technical efficiency by using the same set of weights (common weights) for the efficiency score for all the units. This is in contrast to the DEA efficiency score, which advocates the solution of the linear programming n times, generating a separate set of optimal weight for each unit. The GE involves an optimal solution by one programming for the common set of weights, which maximizes the sum of efficiency scores of all the units. Each efficiency score of the GE with the common weights has the same structure as the DEA efficiency score with the weights that vary from unit to unit; i.e. it is the ratio of total weighted output to total weighted input, bounded by 1. The formulation of the GE is as follows:

$$Z = \max \sum_{j=1}^{n} E_j^*$$

s.t.

$$E_j^* = \frac{\sum_{r=1}^{s} U_r Y_{rj}}{\sum_{i=1}^{m} V_i X_{ij}} \leq 1 \quad j = 1,2,..,\ n$$

$$V_i, U_r \geq 0 \quad i = 1,2,..,\ m \quad r = 1,2,...,\ s$$

The objective function helps the efficiency score with the common weights to reach the DEA scores E_k globally, because by the definition of the DEA, the sum of the DEA scores is the maximum value that any score can reach. The advantage of the GE is its simplicity, the ease with which the average manager may interpret results, and its ranking capabilities according to the common weights that are in the DEA context.

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ON-LINE COST-OPTIMISATION MODEL IN STOCHASTIC PROJECT MANAGEMENT

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Several simultaneously realized activity-on-arc network projects of PERT type with random activity durations are considered. The accomplishment of each project's activity is measured in percentage of the whole project. Any activity entering a project has to be operated by one of the identical comprehensive resource units (CRU) which may use several possible speeds subject to random disturbances. The speeds depend only on the intensity of the project's realization. They are indexed and the number of speeds is common to all CRU.

It is assumed that the progress of any project can be evaluated only via periodical inspections at control points. At any moment $t > 0$ activities that are operated at that moment and which enter one and the same project, have to use speeds with similar indices (ordinal numbers), speeds can be changed only at a control point. Within the projects' realization a CRU can be transferred from one project to another only at the so-called emergency moments common to all projects. The projects' due dates and their chance constraints, i.e., their minimal permissible probabilities of accomplishing the project at its due date, are pregiven. All CRU have to be delivered to the company store when the projects start to be realized, and are released at the moment when the last project is accomplished. The cost of hiring and maintaining a CRU per time unit, together with the average processing costs per time unit for each activity entering each project to be operated under each speed, the average cost of performing a single inspection at the routine control point (common to all projects) and the average cost of reallocating CRU among non-finished projects at each emergency moment, are pregiven.

The newly developed cost-optimisation model is as follows: determine the optimal number of CRU to minimize the total value of all projects' expenses subject to their chance constraints.

Two-level problem's solution is suggested:

- at the company level a combination of a search procedure to determine the number of CPU together with a resource reallocation model among the projects is considered,
- at the project level a cost-optimisation on-line control model is applied for each project independently. This problem has recently been solved in our previous publications.

Keywords: *On-line cost-optimisation problem, Resource reallocation, Project's activity with variable speeds, Non-consumable comprehensive resources*

1. Introduction

Activity-on-arc network projects of PERT type with random activity durations are considered. The progress of each project cannot be inspected and measured continuously, but only at preset inspection points. An on-line control model has to determine both inspection points and control actions to be introduced at those points to alter the progress of the project in the desired direction. Those on-line control models are playing an increasing role in project management. Two different cases may be examined:

A. The network model comprises activities, each of which, being supplied with resources of pregiven capacities, can be operated at one speed only (e.g. PERT-COST projects with budget resources).
B. Each activity can be operated at several possible speeds that are subject to random disturbances and correspond to one and the same resource capacity. That is, these speeds depend only on the degree of intensity of the project's realization (e.g. construction projects where different speeds may correspond to different hours a day per worker). The number of possible speeds is common to all activities. All project activities, being realized between two adjacent control points, have to be operated with speeds of one and the same index.

In both cases cost-optimisation problems can be formulated with different objectives and restrictions. We will consider the second case, where projects under random disturbances with different possible speeds have to be controlled. However, the number of publications on developing on-line control models for stochastic network projects remains very scanty (see, e.g. [1–3]).

The system under consideration comprises several simultaneously realized activity-on-arc network projects of PERT type with random activity durations. The accomplishment of each project's activity is measured in percentage of the whole project. All the activities are to be operated by one of the identical *comprehensive resource units* (CRU) which may use several possible speeds subject to random disturbances. The speeds depend only on the intensity of the project's realization. They are indexed and the number of speeds is common to all CRU.

It is assumed that the progress of any project can be evaluated only via periodical inspection in control points. At any moment $t > 0$ activities that start to operate at that moment for one and the same project, have to use speeds with similar indices (ordinal numbers). Speeds can be changed only at a control point. Within the projects' realization a CRU can be transferred from one project to another only at a so-called emergency moment common to all projects.

The projects' due dates and their chance constraints, i.e., their minimal permissible probabilities of accomplishing the project on time, are pregiven. All CRU have to be delivered to the company store at the projects starting time and are released when the last project is accomplished. The cost of hiring and maintaining a CRU, together with the average processing costs per time unit for operating each activity under each speed, the average cost of performing a single inspection at a control point (common to all projects) and the average cost of reallocating CRU among non-finished projects at each emergency moment, are pregiven.

We have recently formulated and solved a cost-simulation problem for a *single project* as follows: given the *fixed* number of CRU, at each routine control point t_i determine the next control point t_{i+1} and the new index of the speeds for all the activities to be operated at that point. The objective is to minimize the project's total expenses. This basic problem (we will henceforth call it *Problem A1* [4]) will be used in order to develop a much more complicated realistic cost-optimisation model as follows: determine the optimal number of CRU to minimize the total value of all projects' expenses subject to their chance constraints.

The problem's solution is as follows:

- at the company level a combination of a search procedure to determine the number of CRU together with a resource reallocation model among the projects is considered,
- at the project level a basic cost-optimisation on-line control *Model A1* is applied for each project independently.

Both resource reallocation model and *Model A1* are implemented into a simulation model in order to obtain representative statistics to check the fitness of the problem's solution. It is assumed that all non-accomplished projects have to be realized at any moment $t > 0$ with a speed exceeding zero. Thus, at least one CRU unit has to be assigned to each project. At any moment each CRU can operate only one activity.

2. Notation

Let us introduce the following terms:

$G_e(N, A)$ - the e-th network project of PERT type, $1 \le e \le f$;

f - number of network projects with variable speeds;

f_t - number of network projects which at moment t are not completed, $t \ge 0$;

$(i, j)_e \subset G_e(N, A)$ - activity (i, j) entering the e-th project;

G_{et} - project $G_e(N, A)$ observed at moment $t \ge 0$; $G_{e0} = G_e(N, A)$;

$v_{ije}^{(k)}$ - the k-th speed of activity $(i, j)_e$, $1 \le e \le f$, $1 \le k \le m$;

m - number of possible speeds common to all projects and all activities (pregiven);

n_{et} - number of identical generalized resource units CRU assigned to project $G_e(N, A)$ at emergency moment $t \ge 0$; $n_e = n_{e0}$;

n - total number of CRU to be hired and maintained throughout the planning horizon by the company (optimized variable, to be determined beforehand);

ρ_{ije} - percentage of activity $(i,j)_e$ in project $G_e(N,A)$ (pregiven), $1 \le e \le f$;

D_e - due date of project $G_e(N,A)$ (pregiven);

p_e - chance constraint to meet the deadline D_e on time (pregiven);

$V_e^f(t)$ - actual project's G_{et} output in percentages of the total project (observed at moment t, $t \ge 0$);

$C_e^f(t)$ - the actual accumulated processing and control costs of project G_{et} calculated at moment t, $t \ge 0$;

$W_p[t,k,V_e^f(t)]$ - the p-quantile of the moment project $G_e(N,A)$ will be accomplished on condition that the k-th speed for all activities will be introduced at control point t and will be used throughout, and the actual observed output at that moment is $V_e^f(t)$;

t_{ge} - the g-th control point of the e-th project, $g = 0,1,\ldots,N_e$, $t_{0e} = 0$, $t_{N_e e} = D_e$;

t_r^* - the system's emergency moment, $t_0^* = 0$, $r = 0,1,\ldots,N^*$;

N_e - number of control points of the e-th project (a random value);

N^* - number of emergency moments (a random value);

Δ_{1e} - the minimal value of the closeness of the inspection moment to the due date D_e (pregiven);

Δ_{2e} - the minimal time span between two adjacent control points of the e-th project (pregiven);

$t_{ije}^{(k)}$ - random duration of activity $(i,j)_e$ using speed $v_{ije}^{(k)}$ throughout;

$c_{ije}^{(k)}$ - the average processing cost per time unit for activity $(i,j)_e$ to be operated with speed $v_{ije}^{(k)}$ (pregiven);

c_{ins} - the average cost of undertaking a routine project's inspection (common to all projects, pregiven);

c^* - the average cost of the CRU reallocation among the projects at a routine moment t_r^*;

V_e - the planned volume of project $G_e(N,A)$ (pregiven);

V_{et} - the actual non-accomplished volume of project $G_e(N,A)$ at moment t (a random value);

S_{ije} - the actual moment activity $(i,j)_e$ starts (a random value);

F_{ije} - the actual moment activity $(i,j)_e$ is completed (a random value); $F_{ije} = S_{ije} + t_{ije}^{(k)}$;

c_{cru} - the average cost of hiring and maintaining a CRU unit per time unit (pregiven);

F_e - the actual moment project $G_e(N,A)$ is completed (a random value); $F_e = \underset{\{(i,j)_e \in G_{et}\}}{Max} F_{ije}$;

s_{ge} - the index of the speed to be introduced for all activities $(i,j)_e$ starting in the interval $[t_{ge}, t_{g+1,e}]$, $1 \le s_{ge} \le m$.

It can be well-recognized that two kinds of control points are imbedded in the model:

1. *Regular* control (inspection) points t_{ge} to introduce proper speeds in order to alter the project's speed in the desired direction.
2. *Emergency* control points t_r^* to reallocate all CRU at the company level among the non- accomplished network projects, beginning from $t = 0$. Emergency moments t_r^* are as follows:

   $t = 0$;
   t is the moment of one of the project's completion;
   t is the control moment for one of the projects when it is anticipated that with the previously assigned for that project CRU units the project cannot meet its deadline on time.

3. The Problem's Formulation

The cost-optimisation on-line control problem for several stochastic network projects is as follows: determine the optimal value $n^{(opt)}$ of CRU units (a deterministic value to be determined beforehand, i.e., before the projects start to be realized) together with values n_{et} assigned to all projects, all control points t_{ge}, the speeds to be introduced at that points for all projects' activities $v_{ije}^{(k_e)}$, $k_e = s_{ge}$, and the actual moments S_{ije} activities $(i,j)_e$ start (random values conditioned on decision-making of the control model), in order to minimize all operational, control, resource reallocation, hiring and maintenance expenses subject to the projects' chance constraints

$$J = \underset{\left\{n, n_{et}, t_{ge}, S_{ije}, s_{ge}, v_{ije}^{(k)}\right\}}{Min} E\left\{\sum_{e=1}^{f}\sum_{(i,j)_e \in G_{et}}\left(c_{ije}^{(k_e)} \cdot t_{ije}^{(k_e)}\right) + \sum_{e=1}^{f}\left(N_e \cdot c_{ins}\right) + n \cdot c_{cru} \cdot \underset{e}{Max} F_e + N^* \cdot c^*\right\} \quad (1)$$

subject to

$$k_e = s_{ge} \ \forall (i,j)_e : S_{ije} = t_{eg},\ 0 \le g < N,\ 1 \le e \le f, \quad (2)$$

$$Pr\{F_e \le D_e\} \ge p_e,\ 1 \le e \le f, \quad (3)$$

$$t_{0e} = 0,\ 1 \le e \le f, \quad (4)$$

$$t_{N_e} = D_e,\ 1 \le e \le f, \quad (5)$$

$$D_e - t_{ge} \ge \Delta_{1e},\ 0 \le g \le N_e,\ 1 \le e \le f, \quad (6)$$

$$t_{g+1,e} - t_{ge} \ge \Delta_{2e},\ 0 \le g \le N_e,\ 1 \le e \le f, \quad (7)$$

$$s_{ge} \le s_{ge}^* = \underset{1 \le q \le m}{Min}\left\{q : W_p\left[t_{ge}, q, V_e^f\left(t_{ge}\right)\right]\right\}, \quad (8)$$

$$\sum_{e=1}^{f_t} n_{et} = n \text{ for any emergency moment } t \ge 0,\ n_{et} \ge 1. \quad (9)$$

Note that the on-line control model undertakes decision-making either at regular routine control point t_{ge} (determining S_{ije}, $v_{ije}^{(k)}$, $k = s_{ge}$), or at emergency points t_r^* (determining n_{et}, $t = t_r^*$), on the basis of future expenses only, i.e., during the remaining time $D_e - t_{ge}$ (for a single project),

or by taking into account values D_e and p_e, $1 \le e \le f$. Past expenses and past decision-makings are not relevant for the on-line control model. Relation (3) honours the chance constraints. As to relation (8), it refers to the on-line cost-optimisation algorithm for a single project (see [4–5]). Eq. (8) means that the speed to be chosen at any routine control point t_{ge} must not exceed the minimal speed s^*_{ge} that enables meeting deadline D_e on time, subject to be chance constraint p_e. It can be well- recognized that operating an activity at a higher speed always results in higher costs to accomplish the activity than by using a lower speed. Thus, (8) prohibits using unnecessary high speeds. Relation (9) ensures reallocation of n CRU units at the company's disposal among the non-accomplished projects at any emergency moment $t \ge 0$. Relations (4–7) are obvious while (2) ensures assignment of one and the same speed index k_e to all activities which start processing at a routine control point t_{ge}. Note that an activity cannot start at the moment between two adjacent control points t_{ge} and $t_{g+1,e}$.

4. Subsidiary Models

Consider several important subsidiary models which will be used henceforth.

4.1. Subsidiary Model A1

As outlined above, the *basic subsidiary model A1* centres on controlling a single project, without taking into account any resource hiring and maintaining costs. The number of CRU is taken as a fixed and pregiven value. *Model A1* is an on-line cost-optimisation model and is based on the so-called chance constraint principle [3].

The Given average processing costs per time unit for each activity to be operated under each speed, together with the average cost of performing a single inspection at the control point, the problem at a routine control point t_g is to introduce the proper speed $v^{(k)}$ and the next control point t_{g+1}, in order to minimize the total processing costs within the planning horizon, subject to a chance constraint. At each control point, decision-making centers around the assumption that there is no more than one additional control point before the due date. Following that assumption, two speeds $v^{(k_1)}$ and $v^{(k_2)}$ have to be chosen at a routine control point t_g:

1. Speed $v^{(k_1)}$ which has to be actually introduced at point t_g up to the control point t_{g+1};
2. Speed $v^{(k_2)}$ which is forecast to be introduced at control point t_{g+1} up to the due date.

Couple ($v^{(k_1)}, v^{(k_2)}$), which provides the minimal cost expenses, has to be accepted.

The model is mostly effective when each activity can be measured as a partial accomplishment of the whole planned program. The problem is to determine both control points $\{t_g\}$ and activity speeds $\{v_{ij}^{(k)}\}$ to minimize the average project's expenses

$$J = \underset{\{t_g, v_{ij}^{(k)}, s_g\}}{Min} E\left\{ \sum_{(i,j)\in G} \left(c_{ij}^{(k)} \cdot t_{ij}^{(k)}\right) + N \cdot c_{ins} \right\} \tag{10}$$

subject to

$$k = s_g \;\; \forall (i,j): t_g = S_{ij}, \;\; 0 \le g < N, \tag{11}$$

$$Pr\left\{ \underset{\{i,j\}\in G_{t_g}}{Max} \; F_{ij} \le D \right\} \ge p, \tag{12}$$

$$t_0 = 0\,, \tag{13}$$

$$t_N = D\,, \tag{14}$$

$$D - t_g \geq \Delta_1\,,\ 0 \leq g < N\,, \tag{15}$$

$$t_{g+1} - t_g \geq \Delta_2\,,\ 0 \leq g < N\,, \tag{16}$$

$$s_g \leq s_g^* = \underset{1 \leq q \leq m}{Min} \left\{ q : W_p\left[t_g, q, V^f\left(t_g\right)\right] \leq D \right\}. \tag{17}$$

4.2. Subsidiary Model A2

The model differs from *Model A1* by implementing the cost of hiring and maintaining CRU resources within the planning horizon. Thus, objective (10) is substituted by

$$J = \underset{\left\{t_g, v_{ij}^{(k)}, s_g\right\}}{Min}\ E\left\{ \sum_{(i,j)\in G} \left(c_{ij}^{(k)} \cdot t_{ij}^{(k)}\right) + \left(\underset{(i,j)\in G}{Max}\, F_{ij}\right) \cdot n\, c_{cru} + N \cdot c_{ins} \right\} \tag{18}$$

s.t. (11–17),

while the on-line heuristic algorithm remains unchanged.

4.3. Subsidiary Model A3

Determine the minimal number of CRU $n^{(opt)}$ for a single project in order to meet the given chance constraint, i.e.,

$$Min\ n \tag{19}$$

s.t. (11–17).

The Solution

Start ascending value n, beginning from 1. For each n olve *Problem A1* taking into account for each activity (i, j) its *highest speed* $v_{ij}^{(m)}$, i.e., t_{ij} refers to one speed only. Value n, for which relation

$$Pr\left\{ \underset{(i,j)}{Max}\ F_{ij} \leq D \right\} < p\,, \tag{20}$$

ceases to hold, is taken as the solution. Cost parameters are, thus, not taken into account. Denote the optimal number $n^{(opt)}$ by $n(A3)$.

4.4. Subsidiary Model A4

Determine the minimal number of CRU units in order to minimize the objective (18) for the *Model A2* subject to the chance constraint. Thus, two objectives are imbedded in the model

$$Min\ n\,, \tag{21}$$

$$J = \underset{\left\{n, t_g, v_{ij}^{(k)}, s_g\right\}}{Min}\ E\left\{ \sum_{(i,j)\in G} \left(c_{ij}^{(k)} \cdot t_{ij}^{(k)}\right) + \left(\underset{(i,j)\in G}{Max}\, F_{ij}\right) \cdot n\, c_{cru} + N \cdot c_{ins} \right\} \tag{22}$$

s.t. (11–17).

The Solution

Solve *Problem A3* in order to determine value $n(A3)$. Afterwards proceed ascending value n, beginning from $n(A3)$, and for each value $n \geq n(A3)$ solve *Problem A2*. Value $n(A4)$, which delivers the minimum to (22) is taken as the solution of *Problem A4*.

5. The General Idea of the Problem's Solution

The problem (1–9) to be considered (see *Sections 2* and *3*) is a very complicated problem and allows only a heuristic solution. Denote the optimal solution of problem (1–9) by $n(A)$. A basic assertion can be formulated as follows:

Assertion. Let $n_e(A4)$ be the solution of problem A4 for each project $G_e(N, A)$, $1 \leq e \leq f$, independently. Relation

$$n(A) \leq \sum_{e=1}^{f} n_e(A4) = n_{max} \tag{23}$$

holds.

Proof. Any additional CRU unit which results in exceeding value $\sum_{e=1}^{f} n_e(A4)$, has to be assigned to one of the projects $G_e(N, A)$. For that project, as it turns from *Model A4*, the unit becomes redundant. ■

Thus, the general idea of determining $n(A)$ is based on the following concepts:

Concept 1

At the company level the search for an optimal solution is based on examining all feasible solutions $\{n\}$, by decreasing n by one, at each search step, beginning from n_{max}.

Concept 2

Examining a feasible solution centres on simulating the system. Multiple simulation runs have to be undertaken in order to obtain a representative statistics to check the fitness of the model.

Concept 3

A simulation model comprises two-levels. At the higher level – the company level – Sub-algorithm I reallocates n CRU units among f_t non-completed projects at all emergency moments t, beginning from $t = 0$. At the lower level (the project level) Sub-algorithm II undertakes on-line control for each project independently between two adjacent emergency points t_r^* and t_{r+1}^*, by the use of a single-project algorithm of problem A2.

Concept 4

Each value n is examined via M simulation runs to provide a representative statistics to calculate values $Pr\{F_e \leq D_e\}$, $1 \leq e \leq f$, and objective (22).

Concept 5

The search process proceeds by decreasing n by one, i.e., substituting n by $n - 1$, if

all relations $Pr\{F_e \leq D_e\} \geq p_e$, $1 \leq e \leq f$, hold;

value (22) decreases monotonously.

Concept 6

If even for one project $G_e(N, A)$ relation $Pr\{F_e \le D_e\} \ge p_e$ ceases to hold, or value (22) ceases to decrease, the last successful feasible solution n has to be taken as an optimal solution $n(A)$.

6. The Enlarged Procedure of Resource Reallocation (Sub-Algorithm i)

At each emergency point $t \ge 0$ (each emergency point is a control point for all projects as well) reassign n CRU unit among f_t non-accomplished projects as follows:

Step 1. At moment t inspect values V_{et}, $1 \le e \le f$. Note that for already accomplished projects their corresponding values $V_{et} = 0$.

Step 2. By any means reassign n CRU units among f_t projects subject to:

$\sum_e n_{et} = n$;

n_{et} must be whole numbers;

n_{et} must be not less than 1;

relations $n_{et} \ge \left[n \cdot \frac{V_{et}}{\sum_e V_{et}} \right]$, $V_{et} > 0$, $1 \le e \le f$, hold, where $[x]$ denotes the maximum whole number being less than x. Thus, *Step 2* obtains a *non-optimal*, feasible solution.

Step 3. Take value $Z = 10^{17}$, i.e., an extremely large positive value.

Step 4. For all non-accomplished projects G_{et} solve *Problem A2*, independently for each project, with due dates $D_e - t$, chance constraints p_e, resource units n_e and non-accomplished volumes V_{et}. Denote the *actual* probability of meeting the due date on time by $\overline{p}_e$. Values $\overline{p}_e$, $1 \le e \le f$, are obtained via M simulation runs.

Step 5. Calculate values

$$\gamma_e = \frac{\overline{p}_e - p_e}{p_e} \quad , \quad 1 \le e \le f \, .$$

Step 6. Calculate values

$$\gamma_{\xi_1} = \max_e \gamma_e \, ,$$

$$\gamma_{\xi_2} = \min_e \gamma_e \, .$$

Step 7. Calculate $\Delta = \gamma_{\xi_1} - \gamma_{\xi_2}$.

Step 8. If $\Delta < Z$, go to the next step.
Otherwise apply *Step 12*.

Step 9. Set $Z = \Delta$.

Step 10. Transfer one CRU unit from project $G_{\xi_1 t}$ to $G_{\xi_2 t}$, i.e., $n_{\xi_1 t}$ is diminished by one, and $n_{\xi_2 t}$ is increased by one.

Step 11 is similar to *Step 4*, with the exception of solving *Problem A2* for projects $G_{\xi_1 t}$ and $G_{\xi_2 t}$ only. Go to *Step 5*.

Step 12. Values n_{et}, $1 \le e \le f$, which refer to the last successful iteration, are taken as the optimal solution of Sub-algorithm I.

7. The Enlarged Two-Level Heuristic Algorithm of Simulating the System

The enlarged step-by-step procedure of the problem's algorithm is based on simulating the system. The input of the simulation model is as follows:

value $n \ge f$ of CRU units (to be examined by simulation);

pregiven values D_e, p_e, $1 \le e \le f$;

speeds' parameters $v_{ije}^{(k)}$, $(i,j)_e \subset G_e(N,A)$, $1 \le k \le m$;

cost parameters $c_{ije}^{(k)}$, c_{ins}, c_{cru}, c^*;

target parameters V_e, $1 \le e \le f$.

A simulation run comprises the following steps:

Step 1. Set $r = 1$, $t_r^* = 0$.

Step 2. Reallocate at $t = t_r^*$ n CRU units among projects $G_e(N,A)$, $1 \le e \le f$, according to Sub-algorithm I.

Step 3. Reassign values n_{et} obtained at *Step 2*, to projects $G_e(N,A)$.

Step 4. Each project $G_e(N,A)$ is realized independently according to the *Problem A2* (see *Section 4*). In the course of realizing each project any routine control point t_{ge} is examined as follows:

is moment t_{ge} the moment project $G_e(N,A)$ is completed? If yes, go to *Step 9*. Otherwise proceed examining inspection point t_{ge}.

is moment t_{ge} the moment when it is anticipated that project $G_e(N,A)$ cannot meet its deadline on time even by introducing the highest speed with index m? If yes, go to the next step. Otherwise proceed realizing the project until the next routine control point $t_{g,e+1}$.

Step 5. Counter $r + 1 \Rightarrow r$ works.

Step 6. Set $t_r^* = t_{ge}$.

Step 7. Inspect all non-finished projects $G_e(N, A)$ at the routine emergency point t_r^*. Calculate values $V_e^f(t)$, $1 \le e \le f$, $t = t_r^*$.

Step 8. Update all remaining targets $V_e - V_e^f(t) \Rightarrow V_e$, $1 \le e \le f$.
Go to *Step 2* to undertake resource reallocation among non-accomplished projects.

Step 9. Are there at moment $t = t_{ge}$ other, non-accomplished projects? If yes, go to *Step 5*. Otherwise apply the next step.

Step 10. The simulation run terminates.

In the course of carrying out *Steps 2* and *4* the cost-accumulated value J of objective (1) has to be calculated.

The problem's solution is, thus, based on realizing procedures described in *Sections 5–7*.

Conclusions

The following conclusions can be drawn from the study:

1. The developed cost-optimisation simulation algorithm for solving problem (1–9) can be applied to a wide range of project management systems. The outlined model (1–9) enables managing complicated building and construction systems, various R&D systems with different speeds and inspection points, etc.
2. The newly developed on-line control model is a generalized model: it satisfies a variety of chance constraints and develops cost-minimization for a broad spectrum of expenses in the course of the system's functioning.
3. The structure of the algorithm is as follows: at the system's level (the higher level) a search of the optimal number of CRU units is undertaken. At the project's level a basic cost-optimization model for a single project is implemented in the simulation model.
4. The main connection between those two levels is carried out via a newly developed resource reallocation sub-algorithm. The latter is carried out by undertaking probability control to be as close as possible to the projects' chance constraints.

References

1. Golenko-Ginzburg, D., Gonik, A. On-line control model for network construction projects, *Journal of Operational Research Society*, Vol. 48, 1997, pp. 175–183.
2. Golenko-Ginzburg, D., Gonik, A. High performance heuristic algorithm for controlling stochastic network projects, *International Journal of Production Economics*, Vol. 54, 1998, pp. 235–245.
3. Golenko-Ginzburg, D., Gonik, A., Papic, L. Developing cost-optimization production control model via simulation, *Mathematics and Computers in Simulation*, Vol. 49, 1999, pp. 335–351.
4. Golenko-Ginzburg, D., Gonik, A., Sitniakovski, Sh. On-line cost-optimization problem in project management under random disturbances, *Communications in Dependability and Quality Management*, Vol. 4, No 1, 2001, pp. 24–29.
5. Golenko-Ginzburg, D., Laslo, Z., Greenberg, D., Ben-Yair, A. Heuristic "look-ahead" cost-reliability models, *Computer Modelling and New Technologies*, Vol. 12, No 1, 2008, pp. 26–37.

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- **University study**: Moscow physical and technical institute (1968–1974).
- Ph.D. (physics & mathematics) on solid state physics (1982, Physics Institute of Latvian Academy of Sciences), Dr. Sc. Habil (physics & mathematics) on solid state physics (1992, Ioffe Physical Institute of Russian Academy of Sciences).
- **Publications:** 350 publications, 1 patent.
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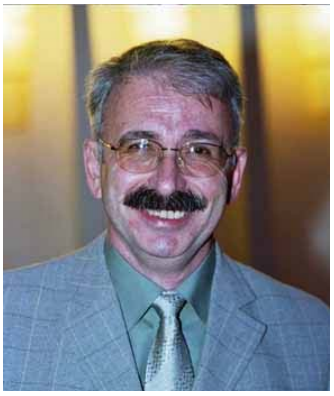

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- Professor-Emeritus and a member of the Paul Ivanier Center on Robotics Research and Production Management, in the Industrial Engineering and Management Department of the Ben-Gurion University of the Negev, Israel, as well as Professor in Department of Industrial Engineering and Management, Ariel University Center in Samaria, Israel
- **Academic and scientific ranks:** Has received M.A. degree in Mathematics from the Moscow State University in 1958 and Ph. D. degree in Applied Mathematics from the Moscow Physical-Technical Institute (Russia) in 1962. In 2007 Prof. Dimitri Golenko-Ginzburg was nominated Honorary Member of the Russian Project Management Association (SOVNET) and elected Foreign Member of the Russian Academy of Natural Sciences, the Branch of Computer Science and Cybernetics.
- **Research activities:** his current research interests are in managing and planning under uncertainty, planning and control of network projects, and industrial scheduling. His professional experience includes 50 years of scientific research and academic teaching in leading academic institutions in the former USSR and, after repatriating in 1985, in Israel.
- **Publications:** In Russia during the period 1958÷1985 he wrote 14 books and more than 200 articles. During the period 1993÷2008 he has been publishing more than 160 articles. His recent publications have appeared in Mathematics and Computers in Simulation, International Journal of Production Economics, Automation and Remote Control, Communications in Dependability and Quality Management, Journal of Applied Quantitative Methods, and Computer Modelling and New Technologies.

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- Senior Lecturer in the Industrial Engineering and Management Department, Sami Shamoon College of Engineering, Israel.
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- **Scientific interests:** His current research interests are in economic aspects of safety, reliability and failure analysis, trade-off optimisation models for organization systems, production planning, scheduling and control, cost optimisation and PERT-COST models, and strategic management.
- **Publications:** He has published about 50 articles in various scientific sources. His recent publications are in Mathematics and Computers in Simulation, International Journal of Production Economics, Communications in Dependability and Quality Management, Journal of Applied Quantitative Methods, and Computer Modelling and New Technologies.

Doron Greenberg

- Senior Lecturer and Head of the financial branch of the Department of Economics and Business Administration in the Ariel University Center (AUC). He is also the 1st Director of the 1st College Chapter of Global Association of Risk Professionals (GARP) in Israel which is affiliated with AUC.
- **Academic and scientific ranks:** Dr. Doron Greenberg earned his doctoral degree in Economics from the University of Houston in 1992; his MBA specialized in Operation Management from the Recanati School of Management in Tel-Aviv (1985); and his B.Sc. in Industrial Engineering from the Technion in Haifa (1980).
- He also has worked as a lecturer in the Recanati School for Management in the Tel-Aviv University, in the Negev College on behalf of Pinchas Sapir, and in the Tel-Aviv College of Engineering. Dr. Greenberg has lectured many courses in Economics and Finance and wrote a dozen of articles in the local newspapers regarding public wealth and finance.
- **Scientific interests:** His main research areas are Economics and Finance. Dr. Greenberg serves currently as Director and Chair of the Investment Committee of the Technical Engineers & Technicians Professional Study Fund in Israel. Dr. Greenberg has reached a profound experience in the Israeli capital market: as a Director and Chair of the Investment Committee of Pension fund of agriculture in Israel, as a financial analyst for institutional investors in Israel, as chairman of Gahelet, a municipal firm which deals with savings for high education, and as a member of the board of directors of PEKAN, one of the top Israeli managing firm of mutual funds. Dr. Greenberg devotes major part of his time and energy to the community. As such he established with other the Israeli chapter of the Transparency International organization (TI), and serves as the CFO of the organization. He also serves as a director in several municipal firms, including: the economic firm of Ariel and the water & sewage firm of Ariel.
- **Publications:** Dr. Doron Greenberg published more than a dozen articles in various scientific branches, including: the Journal of Real Estate Finance and Economics, Communications in Dependability and Quality Management, Technological and Economic Development of Economy, Risk Management, Computer Modelling and New Technologies.

CUMULATIVE INDEX

COMPUTER MODELLING and NEW TECHNOLOGIES, volume 13, No. 1, 2009

(Abstracts)

D. Shapiro, D. Fuks, A. Kiv. Electronic Structure and Chemical Bonding in Laves Phases Al_2Ca, Be_2Ag and Be_2Ti, *Computer Modelling and New Technologies*, vol. 13, No 1, 2009, pp. 7–16.

The results of *ab-initio* calculations of electronic structure of Laves-phase compounds Al_2Ca, Be_2Ag and Be_2Ti are presented. Calculations were carried out in the framework of Density Functional Theory (DFT) and the Full Potential Linearized Augmented Plane Waves + local orbital formalism (FP APW+lo). Total, local and partial densities of electronic states (DOS) were obtained and analysed. These data together with differential electronic density (DED) distribution allow understanding the links of chemical bonding with structural stability of studied compounds.

Keywords: *Laves-phases, ab initio calculations, chemical bonding*

E. K. Shidlovskaya. Cluster Embedding Method for Large Electron Systems: Direct Variational Approach Versus Theory of Pseudopotentials, *Computer Modelling and New Technologies*, vol. 13, No 1, 2009, pp. 17–31.

Problem "cluster in the field of the rest of system" is treated in the frameworks of one-electron approximation with non-orthogonal wave functions. Consideration is general for every task of this type (cluster and the rest of crystal, fragment of a molecule and the remaining part of it, valence and core electrons, etc.). Two alternative approaches are compared:

(A) direct variational approach, when total energy of the whole system (cluster + the rest of system) is expressed in terms of *non-orthogonal* one-electron wave functions and equations for the cluster wave functions are obtained directly from variation of the total energy expression;

(B) approach of the theory of pseudopotentials, when total energy of the system is expressed in terms of *mutually orthogonal* wave functions, equations for the cluster wave functions are obtained under orthogonality constraints and then these equations are transformed to obtain non-orthogonal solutions.

For the both (A) and (B) cases homogeneous equations resulting directly from variational procedure are obtained first. Then these equations are transformed to eigenvalue problem equations. Special case of eigenvalue equations for mutually orthogonal wave functions of the cluster staying to be not orthogonal to the remaining system wave functions is studied. Well-known in the theory of pseudopotentials generalised Phillips-Kleinman (GPK) equations are shown to be particular case of approach (B) eigenvalue equations. Mutually orthogonal wave functions of the cluster are established to be solutions of the equations in the both (A) and (B) cases if additional restrictions on the wave functions are imposed. Unlike theory of pseudopotentials (B), in the case of direct variational approach (A) wave functions of the rest of system are found not to be solutions of the equations for the cluster. It seems to be significant advantage of direct variational approach.

Keywords: *quantum-chemical simulation, embedded molecular cluster (EMC) model, non-orthogonal one-electron wave functions, localised molecular orbitals (LMO), theory of pseudopotentials, generalised Phillips-Kleinman (GPK) equations*

I. Frenkel, A. Lisnianski, L. Khvatskin. Corrective Maintenance and Reliability Associated Cost Estimation of Aging Multi-State Systems, *Computer Modelling and New Technologies*, vol. 13, No 1, 2009, pp. 32–38.

This paper considers corrective maintenance contracts for aging air conditioning systems, operating under varying weather conditions. Aging is treated as an increasing failure rate. The system can fall into unacceptable states for two reasons: through performance degradation because of failures or through an increase in demand of cold. Each residence in acceptable state, each repair and each entrance to an unacceptable state are associated with a corresponding cost. A procedure for computing this reliability associated cost is based on the Markov reward model for a non-homogeneous Poisson process. By using this model an optimal maintenance contract that maximizes the total expected cost may be found. A numerical example for a real world air conditioning system is presented to illustrate the approach.

Keywords: *corrective maintenance, reliability associated cost, aging, multi-state system, Markov reward model*

O. I. Kostyukova, M. A. Kurdina. Properties of Guaranteed Reachable Sets for Linear Dynamic Systems Under Uncertainties with Intermediate Correction Points, *Computer Modelling and New Technologies*, vol. 13, No 1, 2009, pp. 39–48.

In the paper we consider the problem of investigation and constructive description of the reachable sets for linear dynamic systems under unknown but bounded uncertainties over feasible controls that are allowed to be corrected in a given set of correction moments. It is showed that construction of the reachable sets under considered class of feasible uncertainties can be reduced to solving a multilevel min-max optimisation problem with respect to finite dimensional decision variables.

It is proved that adding one new correction moment leads to an extension of the set of system states that can be guaranteed reached at a terminal moment from a given initial position over a feasible control strategy. Numerical example illustrates theoretical results. Some rules for construction external and internal approximations for the reachable sets are discussed.

Keywords: *reachability set, control system, bounded uncertainties*

Y. Hadad, L. Friedman, Z. Sinuany-Stern, A. Ben-Yair. Ranking Method Based on the Difference between Weighted Output and Input, *Computer Modelling and New Technologies,* vol. 13, No 1, 2009, pp. 49–59.

In this paper we developed a new method to establish common weights for measuring the efficiency score of Decision-Making Units (DMUs), based on multiple inputs and multiple outputs. In the new method, these common weights are estimated according to the difference between a weighted sum of outputs and a weighted sum of inputs of the DMUs. We suggest two approaches to rank the DMUs: the first method ranks the DMUs according to the absolute "net profit" (the difference between a weighted sum of outputs and a weighted sum of inputs), while the second method ranks the DMUs according to the relative efficiency score of the ratio between the a weighted sum of outputs and a weighted sum of inputs. In addition we present a method to fix objective bounds for the weights of the variables in the Data Envelopment Analysis (DEA), which is based on the above ranking method. We proved that these bounds are feasible solutions for the DEA methodology. The ranking methods are illustrated on a case study of 24 hospitals in Israel.

Keywords: *Data Envelopment Analysis (DEA), common weights, hospitals*

A. Ben-Yair, D. Golenko-Ginzburg, D. Greenberg. On-Line Cost-Optimisation Model in Stochastic Project Management, *Computer Modelling and New Technologies,* vol. 13, No 1, 2009, pp. 60–69.

Several simultaneously realized activity-on-arc network projects of PERT type with random activity durations are considered. The accomplishment of each project's activity is measured in percentage of the whole project. Any activity entering a project has to be operated by one of the identical comprehensive resource units (CRU) which may use several possible speeds subject to random disturbances. The speeds depend only on the intensity of the project's realization. They are indexed and the number of speeds is common to all CRU.

It is assumed that the progress of any project can be evaluated only via periodical inspections at control points. At any moment $t > 0$ activities that are operated at that moment and which enter one and the same project, have to use speeds with similar indices (ordinal numbers), speeds can be changed only at a control point. Within the projects' realization a CRU can be transferred from one project to another only at the so-called emergency moments common to all projects. The projects' due dates and their chance constraints, i.e., their minimal permissible probabilities of accomplishing the project at its due date, are pregiven. All CRU have to be delivered to the company store when the projects start to be realized, and are released at the moment when the last project is accomplished. The cost of hiring and maintaining a CRU per time unit, together with the average processing costs per time unit for each activity entering each project to be operated under each speed, the average cost of performing a single inspection at the routine control point (common to all projects) and the average cost of reallocating CRU among non-finished projects at each emergency moment, are pregiven.

The newly developed cost-*optimisation* model is as follows: determine the optimal number of CRU to minimize the total value of all projects' expenses subject to their chance constraints.

A two-level problem's solution is suggested:

- at the company level a combination of a search procedure to determine the number of CPU together with a resource reallocation model among the projects is considered,
- at the project level a cost-*optimisation* on-line control model is applied for each project independently. This problem has recently been solved in our previous publications.

Keywords: *On-line cost-optimisation problem, Resource reallocation, Project's activity with variable speeds, Non- consumable comprehensive resources.*

COMPUTER MODELLING and NEW TECHNOLOGIES, 13.sējums, Nr. 1, 2009

(Anotācijas)

D. Šapiro, D. Fuks, A. Kivs. Elektroniskās struktūras un ķīmiskās saiknes laves-fāzēs Al_2Ca, Be_2Ag un Be_2Ti, *Computer Modelling and New Technologies,* 13.sēj., Nr.1, 2009, 7.–16. lpp.

Rakstā tiek piedāvāti Laves-fāzes savienojumu Al_2Ca, Be_2Ag un Be_2Ti elektronisko struktūru *ab-initio* aprēķinu rezultāti. Aprēķini tika veikti *Density Functional Theory (DFT)* un *Full Potential Linearized Augmented Plane Waves* + lokālo orbitālu formālisms (*FP APW+lo*) ietvaros. Vispārējie, vietējie un daļējie elektronisko stāvokļu blīvumi ir iegūti un analizēti. Šie dati kopā ar atšķirīgo elektronisko blīvuma sadalījumu ļauj izprast ķīmisko savienojumu saites ar izskatīto savienojumu strukturālo stabilitāti.

Atslēgvārdi: *Laves-fāzes, ab-initio aprēķini, ķīmiskie savienojumi*

E. K. Shidlovskaya. Klasteru iestiprināšanas metode lielajām elektroniskajām sistēmām: tieša variācijas pieeja pret pseidopotenciāļu teoriju, *Computer Modelling and New Technologies,* 13.sēj., Nr.1, 2009, 17.–31. lpp.

Problēma „klasteris atlikušās sistēmas jomā" tiek diskutēta viena-elektrona aproksimācijas ar ne-ortogonāla viļņa funkcijām ietvaros. Apsvērums ir vispārējs ikvienam šī tipa uzdevumam (klasteris un kristāla atlikums, molekulas fragments un tā atlikusī daļa, etc.). Divas alternatīvas pieejas tiek salīdzinātas.

(A) tiešā variāciju pieeja, kur kopējā visas sistēmas enerģija (klasteris + sistēmas atlikums) tiek izteikta ar ne-ortogonāla viena elektrona viļņa funkcijām, un klasteru viļņa funkciju vienādojumi tiek iegūti tieši no kopējās enerģijas izpausmes variācijas;

(B) pseido-potenciāļu teorijas pieeja, kad sistēmas kopējā enerģija tiek izteikta ar savstarpējās ortogonalitātes viļņa funkcijām, un klasteru viļņa funkciju vienādojumi tiek iegūti ortogonalitātes spaidu kārtā un tad šie vienādojumi tiek pārveidoti, lai iegūtu ne-ortogonālos risinājumus.

Pirmām kārtām abos gadījumos kā (A), tā arī (B) gadījumā tiek iegūti viendabīgi vienādojumi, kas izriet tieši no variāciju procedūras. Pēc tam šie vienādojumi tiek pārveidoti pašvērtību problēmu vienādojumos.

Pētījumā tiek parādīta tiešās variāciju pieejas priekšrocības.

Atslēgvārdi: *quantum-ķīmiska simulācija, iestiprinās molekulārs klastera modelis, ne-ortogonāla viena elektrona viļņa funkcijas, vispārināti Phillips-Kleinman vienādojumi*

I. Frenkels, A. Lisnjanski, L. Hvatkins. Korektīva apgādība un uzticamība saistītais izmaksu vērtējums multi-stāvokļu sistēmu nolietojamībai, *Computer Modelling and New Technologies,* 13.sēj., Nr.1, 2009, 32.–38. lpp.

Šajā rakstā tiek izskatīti korektīvie apgādības līgumi gaisa kondicionēšanas sistēmu, kuras darbojas dažādos laika apstākļos, nolietojamības gadījumiem. Sistēmai var iestāties nepieņemami stāvokļi divos gadījumos: darbības degradācijas bojājumu dēļ, vai arī aukstuma palielināšanās dēļ. Jebkurš gadījums prasa zināmas izmaksas. Ar uzturēšanu saistītā aprēķinu procedūra ir pamatota uz Markova atlīdzības modeli nehomogēnam Puasona procesam. Lietojot šo modeli, optimāls uzturēšanas līgums, kurš palielina kopējās paredzamās izmaksas, var tikt rasts. Rakstā tiek parādīti arī skaitliski piemēri.

Atslēgvārdi: *korektīvā uzturēšana, nolietojamība, ar uzticamību saistītās izmaksas, multi-stāvokļu sistēma, Markova atlīdzības modelis*

O. Kostjukova, M. Kurdina. Garantēto sasniedzamo rindu īpašības lineārām dinamiskām sistēmām pie nejaušībām ar korekciju starppunktiem, *Computer Modelling and New Technologies,* 13.sēj., Nr.1, 2009, 39.–48. lpp.

Rakstā autori izskata izpētes problēmu un dod konstruktīvu aprakstu par sasniedzamām rindām lineārām dinamiskām sistēmām pie nezināmām, bet saistītām nejaušībām pār iespējamo kontroli, kas tiek atļautas būt labotas dotajā korekciju momentu rindā. Tiek parādīts, ka sasniedzamo rindu veidošana pie izskatītās iespējamo nejaušību klases var būt reducēta uz daudzlīmeņu min-max optimizācijas problēmu sakarā ar ierobežotiem dimensionāliem lēmumu mainīgajiem risinājumu.

Tiek pierādīts, ka viena jauna korekcijas momenta pievienošana ved pie sistēmas stāvokļu rindas paplašinājuma, kas var būt garantēti sasniegts terminētā momentā no dotās sākuma pozīcijas pār iespējamo kontroles stratēģiju. Skaitliskie piemēri ilustrē teorētiskos rezultātus. Dotajā rakstā tiek diskutēti daži likumi sasniedzamo rindu ārējo un iekšējo aproksimāciju veidošanai.

Atslēgvārdi: *sasniedzamības rinda, kontroles sistēma, saistītās nejaušības*

J. Hadads, L. Fridmans, Z. Sinuani-Sterns, A. Ben-Jears. Rindu metode, pamatota uz atšķirību starp svērto izlaidi un ieguldījumu, *Computer Modelling and New Technologies,* 13.sēj., Nr.1, 2009, 49.–59. lpp.

Šajā rakstā autori izstrādā jaunu metodi, lai ieviestu kopēju vērtēšanu Lēmumu Pieņemšanas Vienību (*Decision-Making Units (DMUs)*) efektivitātes punktu noteikšanai, kas pamatojas uz daudzkārtīgiem ieguldījumiem un daudzkārtīgu izlaidi. Jaunajā metodē šī kopējā svēršana tiek noteikta saskaņā ar atšķirībām starp *DMUs* izlaides svērto summu un ieguldījumu svērto summu. Autori piedāvā divas pieejas *DMUs* sarindošanai: pirmā metode sarindo *DMUs* saskaņā ar absolūto „tīro peļņu", bet otrā metode sarindo *DMUs* saskaņā ar relatīvās efektivitātes punktu proporciju starp izlaides svērto summu un ieguldījumu svērto summu. Pielikumā autori dod metodi, lai fiksētu objektīvos ierobežojumus mainīgo lielumu svēršanai Datu Apiešanas Analīzē (*Data Envelopment Analysis (DEA)*), kas pamatojas uz iepriekšējo rindas metodi. Autori pierāda, ka šie ierobežojumi ir iespējami risinājumi *DEA* metodoloģijai. Rindu metodes tiek ilustrētas pēc 24 Izraēlas slimnīcu stāvokļu izpētes.

Atslēgvārdi: *Datu Apiešanas Analīze (DEA), kopējā svēršana, slimnīcas*

A. Ben-Jears, D. Golenko-Ginzburgs, D. Grīnbergs. Izmaksu optimizācijas modelis tiešsaistē stohastiskajā projektu vadīšanā, *Computer Modelling and New Technologies,* 13.sēj., Nr.1, 2009, 60.–69. lpp.

Daži vienlaikus realizētie darbība-*on-arc PERT* tipa tīkla projekti ar nejaušiem aktivitāšu ilgumiem tiek izskatīti dotajā rakstā. Katra projekta darbības pabeigšana tiek vērtēta visa projekta procentuālajā izteiksmē. Ikvienai darbībai, kas iekļautas projektā, ir jābūt darbinātai ar vienu no identiskajām vispusīgajām resursu vienībām (*comprehensive resource units (CRU)*), kas var lietot dažus iespējamos ātrumus, pakļautus nejaušiem nemieriem. Ātrumi ir atkarīgi tikai no projekta realizācijas intensitātes. Tie tiek indeksēti un ātruma skaitlis ir kopējs visām *CRU*.

Tiek pieņemts, ka ikviena projekta progress tiek vērtēts tikai caur periodiskām apskatēm kontroles punktos. Ikvienā momentā $t > 0$ darbības, kas notiek šajā momentā un kuras iekļaujas vienā un tajā pašā projektā, tām ir jālieto ātrumi ar līdzīgiem rādītājiem (kārtas skaitlis) un ātrumi var būt mainīti tikai kontroles punktos. Projekta realizēšanas laikā *CRU* var tikt pārvietotas no viena projekta otrā tikai tā saucamajos neparedzētajos gadījumos, kas ir kopēji visiem projektiem.

Jaunatklātais izmaksu optimizācijas modelis ir šāds: nosaka optimālo *CRU* skaitli, lai samazinātu visu projektu izmaksu kopējo vērtību, kas pakļauta to iespējamajiem ierobežojumiem.

Divlīmeņu problēmas risinājumam tiek piedāvāts:

- ir izskatīta uzņēmuma līmenī pētīšanas procedūras kombinācija, lai noteiktu *CRU* skaitli kopā ar resursu asignējumu modeli starp projektiem;
- projektu līmenī izmaksu optimizācijas kontroles modelis tiešsaistē tiek pielietots katram projektam atsevišķi. Šī problēma pavisam nesen tika atrisināta dotā raksta autoru publikācijās.

Atslēgvārdi: *optimizācijas kontroles modelis tiešsaistē, resursu asignējums, projektu darbība ar mainīgiem ātrumiem, nepielietojamie vispusīgie resursi*

COMPUTER MODELLING & NEW TECHNOLOGIES

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