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Highlights

Over 10 years of experience in theoretical modeling of chemical systems. Simulation of complex non-linear chemical reactions. Developing of atmospheric chemical models. Investigation of complex oscillation and chaos behaviour. Quantum chemical studies of reaction mechanisms.

Education background

Ph.D, Physical Chemistry, 2000
Institute of Organic Chemistry, Ufa Research Center, Russian Academy of Science
Thesis: "[An investigation of complex dynamics of chemical systems by the methods of mathematical modeling](#)"

Models of the Belousov-Zhabotinsky reaction were developed and studied using created programming tools. In particular, regions of oscillations existence and routes to chaos were investigated. Full bifurcation diagram of the system was constructed.

MS, Physical Chemistry, 1996
[Chemical Department, Bashkir State University](#)
Thesis: "Development and approbation of the program for solution of inverse kinetic problem"
Software package for chemical reactions simulation and kinetic parameters fitting was developed. It was used to estimate reactions rate constants of radical decay reaction of cyclohexanesulfochloride in presence of molecular oxygen.

Professional experience

2009, Contractor
[Environment Canada](#), Air Quality Modelling and Integration Section
Developing of **GRAHM** mercury atmospheric model, particularly soil and oceanic models, gas and liquid phase chemistry.

2008, Research Associate
[Departments of Atmospheric and Oceanic Sciences, McGill University](#)
Development of **BIRA-IGCM** chemical global circulation model and **FASTOC** (Fast Stratospheric Ozone Chemistry scheme) to represent the full stratospheric chemistry. Evaluation of the CGCM.

2006-2007, System administrator
[Departments of Atmospheric and Oceanic Sciences, McGill University](#)
Adaptation, compilation, installation and support of various atmospheric chemistry and

dynamics models, such as [GEM](#), [IGCM](#), [LAGRANTO](#), [MECCA](#). Developing of conversion programs between the following data file formats: [GRIB](#), [NetCDF](#), [FST](#).

2006, Research assistant

[Departments of Atmospheric and Oceanic Sciences](#), [McGill University](#)

Study of atmospheric reactions of aromatic compounds with chlorine atoms, mercury complexes with water and ozone by quantum chemical methods.

2001-2005, Postdoctoral researcher

[Departments of Atmospheric and Oceanic Sciences](#) and [Chemistry](#), [McGill University](#)

Quantum chemical investigation of atmospheric reactions of carbonyl oxides with water and water clusters. Modeling of tropospheric reactions of mercury, sulfur oxidation in aerosols.

1999 – 2000, Lecturer

[Ufa State Petroleum Technical University](#)

Teach courses: "Numerical methods", "Basics of computing", "Pascal programming language".

Research interest and experience

- Modeling and investigation of complex chemical processes.
- Atmospheric chemical models development.
- Quantum chemical investigation of chemical reactions.
- Inverse kinetic problem – theory and practice.

Skills

Programming languages: Fortran 77/90/95, C/C++, Pascal, Python, x86 assembler, UNIX scripting tools (bash, csh, ksh, awk, sed, etc), [SVL](#)

Compilers and developer tools: GCC, PGI, Intel compilers, SVN, Visual Studio, Borland Delphi, C++ Builder, Waterloo Maple, Free Pascal

Operating Systems: Linux (SUSE, RedHat, Debian), UNIX (Tru64, AIX, IRIX), Windows

Atmospheric models: [GEM](#), [IGCM](#), [Lagranto](#) and data formats: [GRIB](#), [NetCDF](#), [RPN standard file format](#)

Packages for quantum-chemical calculations: [GAMESS](#), [Gaussian 94/98/03](#), [MOLPRO](#), [HyperChem](#), [Jaguar](#), [MOPAC](#), [WinMopac](#), [MOE](#)

Programs for data processing: [Jandel SigmaPlot](#), [Golden Software Grapher and Surfer](#), [Ferret](#)

Experience in computer data acquisition, 3D visualization ([OpenGL](#)), parallel programming ([OpenMP](#) and [MPI](#)), computer hardware, networks and Internet technologies

Packages for analysis of non-linear reaction mechanisms: [AUTO](#), [LOCBIF](#)

Office and desktop publishing software: [MS Office](#), [Corel Draw](#), [Adobe Photoshop](#)

Citizenship

Canada and Russian Federation

My Software

ViewMol3D: 3D OpenGL viewer for molecular structures from the output of quantum chemistry calculations: <http://redandr.ca/vm3>

BZPhase4D: program for modelling of the Belousov-Zhabotinsky reaction and building of 3D/4D phase portraits: <http://redandr.ca/BZPhase.htm>

Kinetic Systems Solver: program for simulation of complex chemical reaction kinetics, including complex and stiff systems: <http://redandr.ca/kss>

FST2CDF: converter of the Standard RPN files (FST), usually output files of the GEM, to the NetCDF format.

<https://www.meteo.mcgill.ca/hydroxyl/wiki/doku.php?id=internal:fst2cdf>

CDF2FST: to transfer data from NetCDF files to Standard RPN format (FST), usually used to prepare data for the GEM.

<https://www.meteo.mcgill.ca/hydroxyl/wiki/doku.php?id=internal:cdf2fst>

GRIB2CDF: GRIB to NetCDF converter to extract data from [ERA15](#) and [ERA40](#) data sets. <https://www.meteo.mcgill.ca/hydroxyl/wiki/doku.php?id=internal:grib2cdf>

Other programs: <http://redandr.ca>

Interests

Wikipedia, Photography, Computer hardware.

Selected publications

A.B. Ryzhkov, H. Niki, G.W. Harris, F. Raofie, P.A. Ariya, Chapter 13 “[Theoretical and Experimental Studies of the Gas-Phase Cl-Atom Initiated Reactions of Benzene and Toluene](#)”, *Advances in Quantum Chemistry (55), Applications of Quantum Chemistry to the Atmosphere (2008)*, 275-295

M.R. Talipov, A.B. Ryzhkov, S.L. Hursan, R.L. Safullin, “[Theoretical investigation of the electronic spectra of aromatic nitrosooxides with allowance for solvent effects](#)”, *Journal of Structural Chemistry*, 2006, 47(6), 1051-1058

S. A. Grabovskiy, E. A. Markov, A. B. Ryzhkov and N. N. Kabal'nova, “[Products, kinetic regularities, and mechanism of thermal decomposition of ethyl \(methyl\) dioxirane](#)”, *Russian Chemical Bulletin*, 2006, 55(10), 1780-1787

A.B. Ryzhkov, P.A. Ariya. "[The importance of water clusters \$\(\text{H}_2\text{O}\)_n\$ \(\$n = 2, \dots, 4\$ \) in the reaction of Criegee intermediate with water in the atmosphere](#)", *Chemical Physics Letters*, 2006, 419, 479-485

P.A. Ariya, A.P. Dastoor, M. Amyot, W.H. Schrieder, L. Barrie, K. Anlauf, F. Raofie, A. Ryzhkov, D. Davignon, J. Lalonde, A. Steffen. "[The Arctic: a sink for mercury](#)", *Tellus B, Chemical and Physical Meteorology*, 2004, 56 (5), 397-403

A. Ryzhkov, P.A. Ariya. "[A theoretical study of the reactions of parent and substituted Criegee intermediates with water and the water dimer](#)", *Phys. Chem. Chem. Phys.*, 2004, 6 (21), 5042-5050

P.A. Ariya, A. Ryzhkov. "[Atmospheric transformation of elemental mercury upon reactions with halogens](#)", *J. Phys. IV France* 2003, 107, 57-59

A.B. Ryzhkov, P.A. Ariya. "[A theoretical study of the reactions of carbonyl oxide with water in atmosphere: the role of water dimer](#)", *Chemical Physics Letters* 2003, 367(3,4), 423-429

Recent presentation

Ryzhkov A. "FASTOC II – Further Development of the Fast Stratospheric Ozone Chemistry Scheme", 4th SPARC General Assembly, Bologna, Italy, 31 August - 5 September, 2008

Ryzhkov A.B., Niki H., Harris G.W., Raofie F., Ariya P.A. "Kinetic, product and theoretical studies of the gas-phase reactions of toluene and benzene with chlorine atoms", 89th Canadian Chemistry Conference and Exhibition, Halifax, Canada, May 27-31, 2006

Ryzhkov A.B., Ariya P.A. "Theoretical study of atmospherically important complexes of Criegee intermediate with water clusters and its reactions", 228th American Chemical Society National Meeting, Philadelphia, USA, August 22-26, 2004

Ryzhkov A.B., Ariya P.A. "Structure, stability, and reaction of complexes of Criegee intermediate with water $\text{H}_2\text{COO}-(\text{H}_2\text{O})_n$, $n=1\dots3$: density functional theory investigation", Annual American Physical Society Meeting, Montreal, Canada, March 22-26, 2004

Ryzhkov A.B., Revenaz B.J., Ariya P.A. "Atmospheric impact of alkenes ozonolysis on sulphur oxidation in sulphate aerosols", 10th Annual MAM/GCC Workshop, Atmospheric Physics Group, Toronto, Canada, December 15-16, 2003