THERMODIFFUSION EQUATIONS: LIE SYMMETRY AND EXACT SOLUTIONS

Irina Stepanova

Institute of Computational Modelling, Krasnoyarsk, Russia

Work is supported by RFBR Grant №14-01-31038 and Grant of Science and Technology Support Fund of Krasnoyarsk Territory

Thermal diffusion (Soret) effect

Thermal diffusion (or the Soret effect) is a molecular transport of mass caused by the thermal gradient in a fluid mixture.

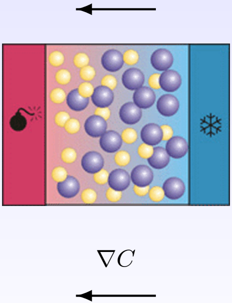
The diffusive flux in a binary mixture is

$$\boldsymbol{J} = -\rho\big(D\nabla C + C(1-C)D_T\nabla T\big).$$

In a closed system at the stationary state and mechanical equilibrium, $\mathcal{J} = 0$, so

$$\nabla C = -C(1-C)\frac{D_T}{D}\,\nabla T.$$

∇T



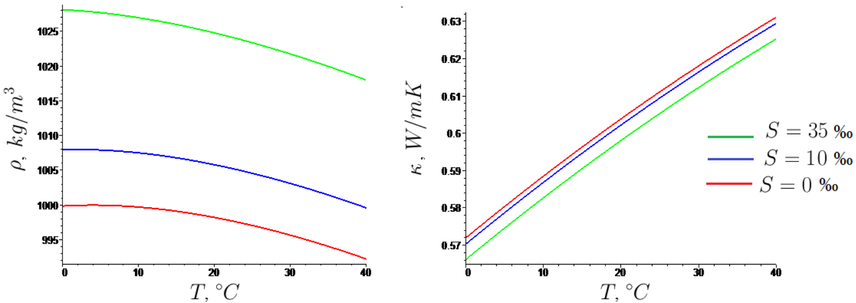
∇C

Transport properties

- density ρ
- viscosity ν
- thermal conductivity κ
- thermal diffusivity χ
- heat capacity c_p
- diffusion coefficient D
- thermal diffusion coefficient D_T

- These are essential to design of chemical processes and equipment involving fluid flow, heat and mass transfer, chemical reactions.
- It is not possible to determine these coefficients by theoretical consideration only. The principle of this study has been the use of mathematical models complemented with some empirical parameters.
- These empirical parameters are determined by comparison between measurements in specially designed experiments and the results of mathematical models that describe the process.

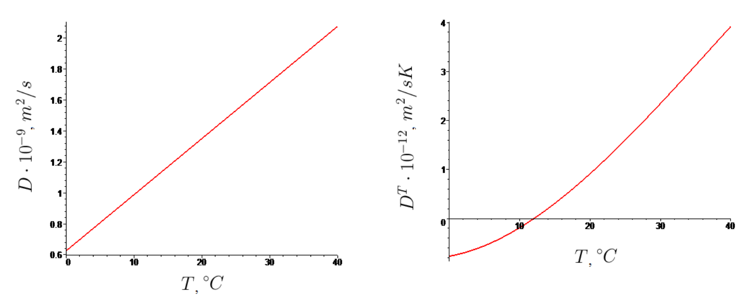
Experimental data (density and thermal conductivity)



Density and thermal conductivity of sea water for different salinity.

M.H. Sharqawy, J.H. Lienhard V, S.M.Zubair *Thermophysical properties of seawater: a review of existing correlation and data*// Desalination and Water Treatment. 16, (2010), 354–380.

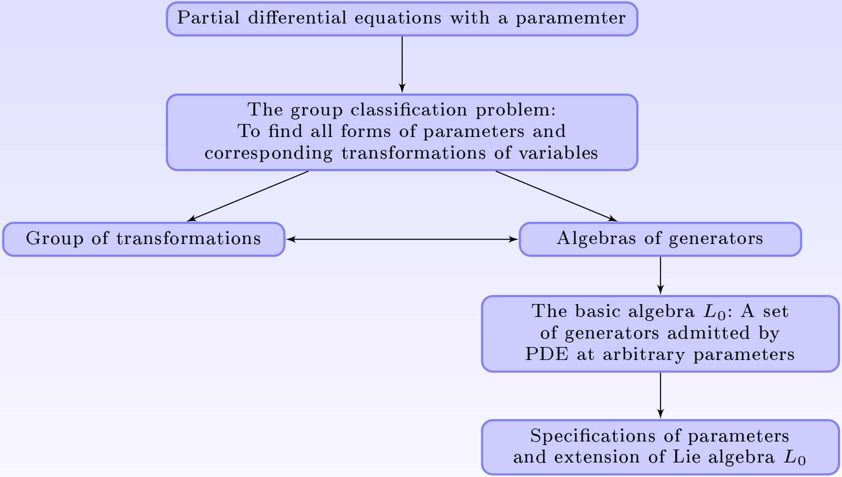
Experimental data(diffusion and thermodiffusion coefficients)



Diffusion and thermal diffusion of NaCl ions in water for salinity 0.0285.

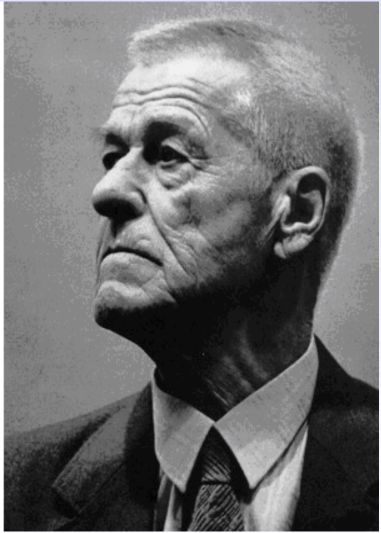
D.R.Caldwell *Thermal and Fickian diffusion chloride in a solution of oceanic concentration*// Deep-Sea Research. 20, (1973), 1029–1039.

The Lie-Ovsyannikov method



- Olver P., *Applications of Lie groups to differential equations*// Springer–Verlag, New York, 1993.
- Ovsyannikov L.V., *Group analysis of differential equations*// Academic Press, New York, 1982.

Lev Vasilyevich Ovsyannikov (1919-2014)



- Academician L.V. Ovsyannikov is an outstanding Russian scientist, who made a great contribution to the development of mechanics and applied mathematics.
- His works have generated the beginning of new research fields, actively developing in Russia and over the world.
- The results of Ovsyannikov in gas dynamics, the theory of fluid motion with free boundaries in the field of mathematical study models of continuum mechanics have become classical.
- L.V. Ovsyannikov is one of the founders of the group analysis of differential equations. All his paper features a clear statement of the problem, elegant and rigorous mathematical apparatus.

Application of symmetry analysis to convection equations

- Stepanova I. V. *Symmetry analysis of nonlinear heat and mass transfer equations under Soret effect.* Commun Nonlinear Sci Numer Simulat, 2015. V. 20.
- Stepanova I. V. *Group classification for equation of thermodiffusion in binary mixture.* Commun Nonlinear Sci Numer Simulat, 2013. V. 18.
- Ryzhkov I. I. *Symmetry analysis of equations for convection in binary mixture.* Journal of Siberian Federal University. Mathematics and Physics, 2008. V. 1(4).
- Andreev V. K., Stepanova I. V. *Symmetry of thermodiffusion equations under nonlinear dependence of buoyancy force on temperature and concentration.* Computational Technologies Journal, 2010. V. 15(4) (in Russian).
- Goncharova O. N. *Group classification of the free convection equations.* Continuum dynamics: collection of papers, Novosibirsk 1987. V. 79 (in Russian).

Heat and mass transfer equations under Soret effect

$$\frac{\partial T}{\partial t} = \chi\left(\frac{\partial^2 T}{\partial (x^1)^2} + \frac{\partial^2 T}{\partial (x^2)^2} + \frac{\partial^2 T}{\partial (x^3)^2}\right) + \\ + \frac{\partial \chi}{\partial T}\left(\left(\frac{\partial T}{\partial x^1}\right)^2 + \left(\frac{\partial T}{\partial x^2}\right)^2 + \left(\frac{\partial T}{\partial x^3}\right)^2\right) + \\ + \frac{\partial \chi}{\partial C}\left(\frac{\partial T}{\partial x^1}\frac{\partial C}{\partial x^1} + \frac{\partial T}{\partial x^2}\frac{\partial C}{\partial x^2} + \frac{\partial T}{\partial x^3}\frac{\partial C}{\partial x^3}\right), \tag{1}$$

$$\frac{\partial C}{\partial t} = D\left(\frac{\partial^2 C}{\partial (x^1)^2} + \frac{\partial^2 C}{\partial (x^2)^2} + \frac{\partial^2 C}{\partial (x^3)^2}\right) + \frac{\partial D}{\partial T}\left(\frac{\partial T}{\partial x^1}\frac{\partial C}{\partial x^1} + \frac{\partial T}{\partial x^2}\frac{\partial C}{\partial x^2} + \frac{\partial T}{\partial x^3}\frac{\partial C}{\partial x^3}\right) + \\ + \frac{\partial D}{\partial C}\left(\left(\frac{\partial C}{\partial x^1}\right)^2 + \left(\frac{\partial C}{\partial x^2}\right)^2 + \left(\frac{\partial C}{\partial x^3}\right)^2\right) + D_T\left(\frac{\partial^2 T}{\partial (x^1)^2} + \frac{\partial^2 T}{\partial (x^2)^2} + \frac{\partial^2 T}{\partial (x^3)^2}\right) + \\ + \frac{\partial D_T}{\partial T}\left(\left(\frac{\partial T}{\partial x^1}\right)^2 + \left(\frac{\partial T}{\partial x^2}\right)^2 + \left(\frac{\partial T}{\partial x^3}\right)^2\right) + \frac{\partial D_T}{\partial C}\left(\frac{\partial T}{\partial x^1}\frac{\partial C}{\partial x^1} + \frac{\partial T}{\partial x^2}\frac{\partial C}{\partial x^2} + \frac{\partial T}{\partial x^3}\frac{\partial C}{\partial x^3}\right), \tag{2}$$

References

- *L.V.Ovsyannikov*, Group properties of nonlinear thermal conductivity equations, *Doklady AS USSR*, **125** 3 (1959) 492-495.

$$\partial_t u = \partial_x(\theta(u)\partial_x u)$$

- *N.M. Ivanova and C. Sophocleous*, On the group classification of variable-coefficient nonlinear diffusion-convection equations, *J. Comput. Appl. Math.* **197** (2006) 322-344.

$$f(x)u_t = (g(x)D(u)u_x)_x + K(u)u_x$$

- *I.B. Kovalenko and A.G. Kushner*, The non-linear diffusion and thermal conductivity equation: group classification and exact solutions, *Regular and Chaotic Dyn.* **8** (2003) 167–189.

$$u_t = (u^\alpha u_x)_x + F(u)$$

The basic group and additional generators

$$L^0 = \langle \partial_t,\ \partial_{x^i},\ 2t\partial_t + \sum_{i=1}^{3} x^i \partial_{x^i},\ x^j \partial_{x^i} - x^i \partial_{x^j} \rangle,\ i, j = 1, ..., 3,\ i \neq j.$$

generator	transformation
∂_t	time transition
$\partial_{x^i},\ i = 1, \ldots, 3$	space transition
$x^j \partial_{x^i} - x^i \partial_{x^j},\ i, j = 1, ..., 3,\ i \neq j$	rotation
$2t\partial_t + \sum_{i=1}^{3} x^i \partial_{x^i}$	scale transformation

Additional generators

$$Z = (m + n)\left(t\partial_t + \sum_{i=1}^{3} x^i \partial_{x^i}\right),$$

$$T^1 = T\partial_T,\ T^3 = \partial_T,\ C^1 = C\partial_C,\ C^2 = T\partial_C,\ C^3 = \partial_C.$$

Results of group classification at $\chi = \chi(T, C)$

χ, **D**	$\mathbf{D_T}$	**generators**	**w**
$e^{(m+n)C/T} f_i$	$e^{(m+n)C/T}(C/T(f_1 - f_2) + f_3)$	$Z + C^2$	T
$e^{(m+n)T} f_i$	$e^{(m+n)T}(kT(f_1 - f_2) + f_3)$	$Z + T^3 + kC^2 + qC^3$	$C - kT^2/2 - qT$
$(kT+C)^{m+n} f_i$	$(kT+C)^{m+n}(k(f_2 - f_1) + (kT+C)f_3)$	$Z + kC^2 + C^1$	T
$e^{(m+n)T} f_i$	$e^{(m+n+l)T}(k(f_2 - f_1)e^{-lT} + f_3)$	$Z + T^3 + lkC^2 + lC^1$	$(C + kT + k/l)e^{-lT}$
$T^{m+n} f_i$	$T^{m+n-1}(kT(f_1 - f_2) + f_3)$	$Z + T^1 + kC^2 + qC^3$	$C - kT - q\ln T$
$T^{m+n} f_i$	$T^{m+n}(k(f_2 - f_1)/(h-1) + T^{h-1} f_3)$	$Z + T^1 + kC^2 + hC^1$	$(C + kT/(h-1))T^{-h}$
$T^{m+n} f_i$	$T^{m+n}(k(f_1 - f_2)\ln T + f_3)$	$Z + T^1 + kC^2 + C^1$	$C/T - k\ln T$

Results of group classification at $\chi = \chi_* = \mathrm{const}$

D	$\mathbf{D_T}$	**generators**	**w**
f	$\lambda_2 \ln T(\chi_* - f) + F$	$T^1 + \lambda_2 C^2 + C^1$	$C/T - \lambda_2 \ln T$
f	$\lambda_0 T(\chi_* - f) + F$	$T^3 + \lambda_0 C^2 + \lambda_1 C^3$	$C - \lambda_0 T^2/2 - \lambda_1 T$
f	$C(\chi_* - f)/T + F$	$C^2,\ C^1$	T
f	$\lambda_1(\chi_* - f)/(1 - \lambda_3) + F$	$T^1 + \lambda_1 C^2 + \lambda_3 C^1 + \lambda_1\lambda_2\lambda_3 C^3/(\lambda_3 - 1)$	$(C - \lambda_1(\lambda_2 + T)/(1 - \lambda_3))T^{-\lambda_3}$
f	$\lambda_0(\chi_* - f) + F/T$	$T^1 + \lambda_0 C^2 - \lambda_1 C^3$	$C - \lambda_0 T + \lambda_1 \ln T$
f	$\lambda_1(\chi_* - f) + e^{-\lambda_2 T} F$	$T^3 + \lambda_1\lambda_2 C^2 - \lambda_2 C^1 - \lambda_1 C^3$	$(C + \lambda_1 T)e^{-\lambda_2 T}$

Exact solutions

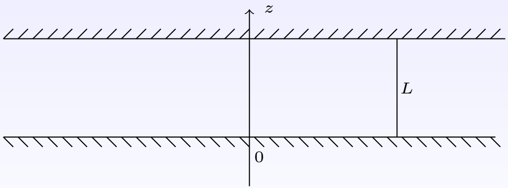
Choose admissible generators

$$\langle \partial_t,\ \partial_{x^1},\ \partial_{x^3} \rangle$$

Choose the transport coefficients

$$\kappa = \kappa(T, C),\ \rho = \rho(T, C),\quad D = D(T, C),\quad D_T = D_T(T, C)$$

Choose the geometry of the problem



Reduced system and boundary conditions

Governing equations:

$$\frac{d}{dz}\left(\kappa(T,C)\frac{dT}{dz}\right) = 0, \tag{3}$$

$$\frac{d}{dz}\left(\rho(T,C)\left(D(T,C)\frac{dC}{dz} + C(1-C)D_T(T,C)\frac{dT}{dz}\right)\right) = 0 \tag{4}$$

Conservation of mass:

$$S'\int_0^{L'} \rho(T,C)\, C\, dz = \rho_0 C_0 S L, \qquad S'\int_0^{L'} \rho(T,C)\, dz = \rho_0 S L, \tag{5}$$

Boundary conditions:

$$T(0) = T_1, \qquad T(L') = T_2, \tag{6}$$

$$\rho(T,C)\left(D(T,C)\frac{dC}{dz} + C(1-C)D_T(T,C)\frac{dT}{dz}\right) = 0 \quad \text{at} \quad z = 0, L'. \tag{7}$$

General solution

Let us integrate governing equations once using boundary condition (5):

$$\kappa(T,C)\frac{dT}{dz} = \kappa_0,$$
$$\frac{dC}{dz} + C(1-C)S_T(T,C)\frac{dT}{dz} = 0,$$

where $S_T(T,C) = D_T/D$ is the Soret coefficient.
To solve the problem, we assume that $z = z(T),\ C = C(T)$:

$$\frac{dz}{dT} = \frac{\kappa(T,C)}{\kappa_0}, \qquad z(T_1) = 0, \qquad z(T_2) = L, \tag{8}$$
$$\frac{dC}{dT} = -C(1-C)S_T(T,C), \qquad C(T_1) = C_1, \tag{9}$$

where C_1 is found from mass conservation conditions (5).
The solution of problem (8) is given by

$$z(T) = \frac{1}{\kappa_0}\int_{T_1}^{T}\kappa\big(\tau, C(\tau)\big)d\tau, \qquad \kappa_0 = \frac{1}{L'}\int_{T_1}^{T_2}\kappa\big(T, C(T)\big)dT. \tag{10}$$

General solution

Consider the problem for concentration C:

$$\frac{dC}{dT} = -C(1-C)S_T(T,C), \qquad C(T_1) = C_1. \tag{11}$$

The mass conservation conditions (5) lead to

$$\int_{T_1}^{T_2} \rho C \kappa \, dT \left(\int_{T_1}^{T_2} \rho\kappa \, dT \right)^{-1} = C_0, \quad \frac{V'}{V} = \rho_0 \int_{T_1}^{T_2} \kappa \, dT \left(\int_{T_1}^{T_2} \rho\kappa \, dT \right)^{-1}, \tag{12}$$

where $C = C(T)$, $\rho = \rho(T, C(T))$, $\kappa = \kappa(T, C(T))$, $V' = S'L'$, $V = SL$.

The general method of solving the problem:

- Solve problem (11) analytically or numerically to find $C(T)$. Determine constant C_1 from first equation in (12).
- Find the dependence of space coordinate on temperature $z(T)$ from

$$z(T) = \frac{1}{\kappa_0} \int_{T_1}^{T} \kappa\big(\tau, C(\tau)\big) d\tau. \tag{13}$$

- Given the functions $z = z(T)$ and $C = C(T)$, determine the temperature and concentration profiles $T(z)$ and $C(z)$.

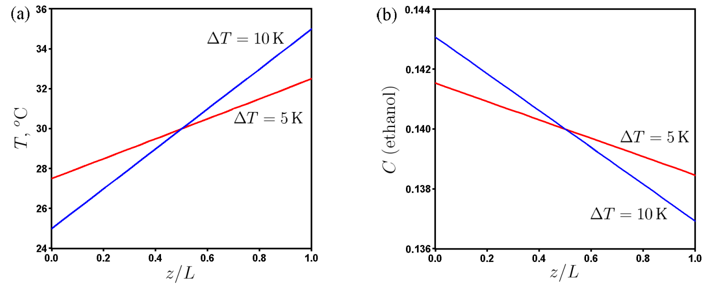
Examples of solution construction

Case 1. Constant ρ, κ and $S_T' = C_0(1 - C_0)S_{T0}$.
The profiles of temperature and concentration are linear:

$$T(z) = T_1 + \frac{T_2 - T_1}{L} z, \tag{14}$$

$$C(z) = C_0 - C_0(1 - C_0)S_{T0}(T_2 - T_1)\left(\frac{z}{L} - \frac{1}{2}\right).$$

Consider ethanol–water mixture at $T_0 = 30^o\mathrm{C}$, $C_0 = 0.14$.
The Soret coefficient is $S_{T0} = 5.11 \cdot 10^{-3}\,\mathrm{K}^{-1}$.



Examples of solution construction

Case 2. Constant ρ, κ and $S_T' = C_0(1 - C_0)S_T(T)$.

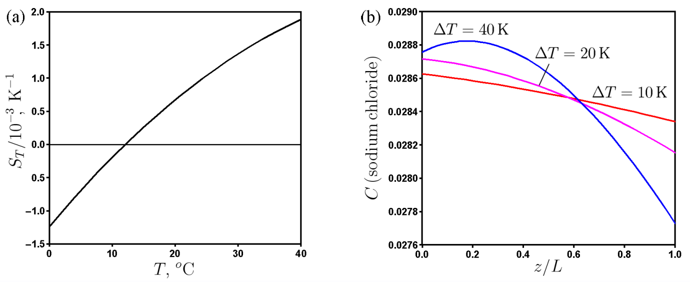
The temperature profile $T(z)$ is linear (see (10)). The general solution for C is

$$C = C_0 - C_0(1 - C_0)\left[\int_{T_1}^{T} S_T(\tau)\,d\tau - \frac{1}{T_2 - T_1}\int_{T_1}^{T_2}\int_{T_1}^{T} S_T(\tau)\,d\tau\,dT\right].$$

For sodium chloride in water near the oceanic concentration $C_0 = 0.0285$

$$S_T = (-1.232 + 0.1128\,T - 0.00087\,T^2)\cdot 10^{-3}\ \mathrm{K}^{-1}.$$

This formula is valid in the range 0–45 ^{o}C. We take $T_0 = 25^o$C.



Examples of solution construction

Case 3. Constant ρ, κ and $S_T' = CS_T(T)$.
For small C, one has $C(1-C) \sim C$.
The temperature profile $T(z)$ is linear (see (14)). The general solution for C:

$$C = C_1 \, \exp\left(-\int_{T_1}^{T} S_T(\tau)\, d\tau \right).$$

After determining C_1 from the condition of mass conservation (first equation in (12)), we find

$$C = \frac{C_0\,(T_2 - T_1)\, \exp\left(-\int_{T_1}^{T} S_T(\tau)\, d\tau \right)}{\int_{T_1}^{T_2} \exp\left(-\int_{T_1}^{T} S_T(\tau)\, d\tau \right) dT}.$$

Examples of solution construction

Consider aqueous suspension of polystyrene spheres

(M. Braibanti, D. Vigolo, R. Piazza, Phys. Rev. Lett. 2008. V. 100, 108303)

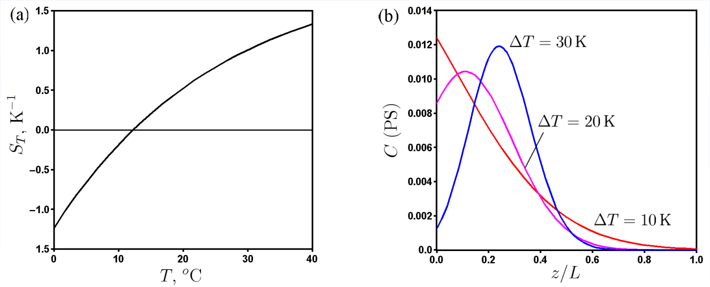
The Soret coefficient in aqueous colloids is written as

$$S_T = S_T^{\infty}\left[1 - \exp\left(\frac{T^* - T}{T_c}\right)\right].$$

For PS spheres with the radius $R = 123$ nm

$$T^* = 12.20\ ^oC, \qquad T_c = 25.63\ K, \qquad S_T^{\infty} = 2.016\ K^{-1}.$$

We take $T_0 = 20^oC$ and initial concentration of PS spheres $C_0 = 0.0035$.



Summary

- The equations describing thermodiffusion without convection in binary mixture with Soret effect under buoyancy force action are considered.
- The Lie symmetries are found. Group classification with respect to the physical parameters is performed.
- Different exact solutions of the governing equations are constructed and analyzed.
- These results are useful for analytical and numerical modeling of heat and mass transfer in binary mixtures with Soret effect.