รหัสโครงการ SUT1-103-54-12-28

รายงานการวิจัย

การสร้างแบบจำลองทางคณิตศาสตร์สำหรับงานประยุกต์ด้านวิทยาศาสตร์และเทคโนโลยี

(Mathematical Modeling for Science and Technology Applications)

ได้รับทุนอุดหนุนการวิจัยจาก

มหาวิทยาลัยเทคโนโลยีสุรนารี

ผลงานวิจัยเป็นความรับผิดชอบของหัวหน้าโครงการวิจัยแต่เพียงผู้เดียว

บทคัดย่อ

โครงการวิจัยนี้ประกอบด้วย 4 งานวิจัยที่เกี่ยวข้องกับการสร้างตัวแบบปรากฏการณ์เชิงกายภาพในงานทางวิทยาศาสตร์ประยุกต์ โดยงานวิจัยดังกล่าวมีส่วนที่เชื่อมโยงกันโดยมีการใช้ระเบียบวิธีที่ประยุกต์ใช้ในฟิสิกส์เชิงคณิตศาสตร์ และคณิตวิเคราะห์ของสมการเชิงอนุพันธ์ในการสร้างตัวแบบ

งานวิจัยที่หนึ่งสามารถแบ่งได้เป็น 3 ส่วนย่อยตามการศึกษาและลำดับการค้นพบดังนี้ สำหรับส่วนย่อยที่หนึ่ง เกี่ยวข้องกับการสร้างตัวแบบทางพลศาสตร์ของไหล โดยในส่วนนี้ได้นำเสนองานประยุกต์อย่างมีระบบของระเบียบวิธีการวิเคราะห์กรุปสำหรับการสร้างตัวแบบของของไหลที่มีความเฉื่อยภายใน และพบว่าโดยการจำแนกกรุปสามารถแบ่งตัวแบบเหล่านี้ได้เป็น 73 คลาส สำหรับส่วนย่อยที่สอง เกี่ยวข้องกับงานประยุกต์ของระเบียบวิธีการวิเคราะห์กรุปของสมการอินทิโกร-ดิฟเฟอร์เรนเชียล งานวิจัยในส่วนนี้เกี่ยวข้องกับการใช้สมการอินทิโกร-ดิฟเฟอร์เรนเชียลแบบอีโวลูชันนารีในการอธิบายสมการคลื่นแบบไม่เชิงเส้น ในงานวิจัยดังกล่าวได้กล่าวถึงการนำเสนอแนวทางใหม่ของการวิเคราะห์กรุปสมัยใหม่และการประยุกต์ใช้ในตัวแบบทั่วไป ซึ่งทำให้ได้สมการที่ถูกลดรูปและผลเฉลยชัดแจ้ง และอีกงานประยุกต์หนึ่งของระเบียบวิธีการวิเคราะห์กรุปของสมการอินทิโกร-ดิฟเฟอร์เรนเชียลนั้นนำไปใช้กับสมการโบลทซ์แมนน์ และได้นำเสนอการจำแนกกรุปสำหรับสมการดังกล่าวเทียบกับแหล่งต้นทางโดยใช้ระเบียบวิธีทางพีชคณิต และสำหรับงานในส่วนย่อยที่สามเป็นการศึกษา 2 ปัญหาคือ ปัญหาอินทิกรัลที่หนึ่งของสมการเชิงอนุพันธ์สามัญอันดับสอง ซึ่งได้นำเสนอถึงอินทิกรัลที่หนึ่งสำหรับตัวแทนเฉพาะที่เกี่ยวข้องกับสมการเชิงอนุพันธ์สามัญอันดับสอง ความสัมพันธ์ระหว่างรูปอินทิกรัล สมการที่เกี่ยวข้อง ความสัมพันธ์สมมูล และตัวอย่างประกอบที่แสดงให้เห็นถึงลักษณะและสมบัติสำคัญต่าง ๆ และปัญหาที่สองเป็นการจำแนกกลุ่มอย่างสมบูรณ์ของระบบสมการของสองสมการเชิงอนุพันธ์สามัญอันดับสองเชิงเส้นที่มีสัมประสิทธิ์เป็นค่าคงตัว ซึ่งได้ปรับแก้วิธีการใช้แบบบัญญัติจอร์ดองในการศึกษาโครงสร้างสมมาตรของระบบสมการของสมการเชิงอนุพันธ์สามัญอันดับสองเชิงเส้นที่มีสัมประสิทธิ์เป็นค่าคงตัวที่นำเสนอโดย Wafo Soh (2010) ให้ถูกต้อง โดยงานวิจัยนี้ได้นำเสนอเพียงระบบสมการที่มีเพียงสองสมการเท่านั้น

งานวิจัยที่สองเกี่ยวกับบริเวณผสมเต็มรูปแบบสองมิติยุบตัวลงในตัวกลางแบบแบ่งเป็นชั้นตามความหนาแน่นอย่างต่อเนื่อง งานวิจัยนี้เป็นการใช้การวิเคราะห์การคำนวณเชิงตัวเลขของพจน์แอดเวกทีฟในสมการนาเวียร์-สโตก ในการประมาณค่าของโอเบอเบค-บัวซิเนสค์ การเปรียบเทียบระหว่างการใช้แผนอับวิน แผนจำกัดค่าฟลักซ์ที่ชื่อว่ามินมอด ซุปเปอร์บี แวนเลียร์ และโมโนโทไนซ์เซนเตอร์ แผนลายฉลุปรับตัวทางเดียวที่ชื่อ ENO3 และ SMIF และแผนลายฉลุถ่วงน้ำหนัก WENO5 ได้ถูกเสนอในงานวิจัยนี้ ข้อมูลการทดลองจากห้องปฏิบัติการของ Wu ได้ถูกนำมาใช้ในการวัดเปรียบเทียบสมรรถนะ เพื่อเปรียบเทียบประสิทธิภาพของแนวทางทางการคำนวณเชิงตัวเลขต่าง ๆ ซึ่งพบว่าแผนจำกัดค่าฟลักซ์จะให้การแพร่เชิงตัวเลขน้อยที่สุด แผน WENO5 ให้ความแม่นยำในการอธิบายความกว้างของบริเวณยุบตัวในเวลาที่แตกต่างกันได้มากกว่า และแผนทั้งหมดที่พิจารณาในงานวิจัยแสดงถึงแบบรูปที่เหมือนจริงสำหรับคลื่นโน้มถ่วงภายในที่ถูกสร้างโดยบริเวณยุบตัว

งานวิจัยที่สามได้พัฒนาแบบจำลองทางคณิตศาสตร์แบบการแปรผันสำหรับการลดสัญญาณรบกวนแบบสเปกเคิลในภาพถ่ายคลื่นเสียงความถี่สูง โดยมีสมมติฐานว่าสัญญาณรบกวนแบบสเปกเคิลมีรูปแบบการแจกแจง

แบบเรย์ลี แบบจำลองทางคณิตศาสตร์ดังกล่าวนำไปสู่การหาค่าน้อยสุดของฟังก์ชันนัลบนปริภูมิของฟังก์ชันของการแปรผันอย่างมีขอบเขต ฟังก์ชันนัลดังกล่าวประกอบด้วยพจน์ของพลังงานและพจน์ของความถูกต้องของข้อมูล ซึ่งได้มาจากการแจกแจงแบบเรย์ลี งานวิจัยชิ้นนี้แสดงให้เห็นว่าค่าน้อยสุดของฟังก์ชันนัลมีอยู่จริง และมีอยู่เพียงหนึ่งเดียวภายใต้เงื่อนไขเพิ่มเติมบางประการ ผลเฉลยของสมการออยเลอร์ลากรานจ์ของแบบจำลองทางคณิตศาสตร์ที่ได้ถูกประมาณโดยวิธีเกรเดียนต์เดสเซนต์ ในส่วนของการทวนสอบความถูกต้องของแบบจำลอง ภาพที่มีลักษณะเป็นแบบรูปและภาพของเลนนาได้ถูกนำมาใช้เป็นตัวอย่างการทดสอบ และผลการทำสอบได้ทำการเปรียบเทียบสหสัมพันธ์ระหว่างภาพที่มีสัญญาณรบกวนกับภาพต้นแบบ และภาพที่ถูกบรูณะโดยวิธีต่าง ๆ กับภาพต้นแบบ ผลการศึกษาพบว่าแบบจำลองที่ได้สามารถลดสัญญาณรบกวนจากภาพที่ใช้ทำการทดสอบและวีดิทัศน์ของภาพถ่ายคลื่นเสียงความถี่สูง นอกจากนี้ได้เปรียบเทียบสมรรถนะของการลดสัญญาณรบกวนโดยแบบจำลองที่ได้กับการลดสัญญาณรบกวนโดยแบบจำลองทางคณิตศาสตร์แบบการแปรผันอื่น ๆ อีกด้วย

งานวิจัยที่สี่ได้สร้างแบบจำลองทางคณิตศาสตร์เพื่อใช้ทำนายอัตราการเปลี่ยนรูปผลึกโดยอาศัยสารละลายเป็นสื่อกลางของผลึกที่มีโครงสร้างผลึกมากกว่าหนึ่งแบบ และช่วยให้เข้าใจเรื่อง การเกิดการเปลี่ยนรูปผลึกโดยอาศัยสารละลายเป็นสื่อกลาง มากยิ่งขึ้น ผลการคำนวณที่ได้จากแบบจำลองนี้ได้นำมาเปรียบเทียบกับค่าจากการทดลองการเกิด การเปลี่ยนรูปผลึกโดยอาศัยสารละลายเป็นสื่อกลางของ อัลฟา-ดีแอล-เมทไธโอนีน (α-DL-methionine) ไปเป็นแกมมา-ดีแอล-เมทไธโอนีน (γ-DL-methionine) โดยเปรียบเทียบในส่วนของความเข้มข้นของเมทไธโอนีนที่เปลี่ยนแปลงไปตามเวลาและอัตราส่วนโดยมวลของผลึกทั้งสองแบบ เบื้องต้นนั้นตัวแปรต่าง ๆ ที่ใช้ในการสร้างแบบจำลองเจาะจงใช้เฉพาะที่สามารถวัดได้จากการทดลองเกี่ยวกับปรากฏการณ์ การโตของผลึก การเกิดผลึกใหม่ การละลายของผลึก และช่วงเวลาก่อนการเกิดผลึกของผลึกทั้งสองแบบ โดยไม่มีตัวแปรที่สร้างมาจากข้อมูลของการเปลี่ยนรูปผลึกโดยอาศัยสารละลายเป็นสื่อกลางมาเกี่ยวข้อง ซึ่งแบบจำลองที่สร้างขึ้นให้ผลการคำนวณไปในทิศทางเดียวกันกับข้อมูลที่ได้จากผลการทดลอง แต่ค่าอัตราการเปลี่ยนแปลงโครงสร้างของผลึกนั้นไม่ถูกต้อง จากการวิเคราะห์ผลที่ได้ทำให้ทราบว่าตัวแปรที่มีผลทำให้แบบจำลองและการทดลองให้ผลไม่เหมือนกันคือ ค่าคงที่ของอัตราการละลาย เนื่องจากเมื่อลองกำหนดตัวแปรที่เกี่ยวข้องกับข้อมูลการเกิดการเปลี่ยนรูปผลึกโดยอาศัยสารละลายเป็นสื่อกลาง เพิ่มลงไป แบบจำลองให้ผลออกมาดีมาก สำหรับเหตุผลของความคลาดเคลื่อนของแบบจำลองนั้นก็ได้วิเคราะห์และนำเสนอไว้ในงานวิจัยนี้แล้ว การศึกษาในส่วนที่สองเป็นการสร้างแบบจำลองทางคณิตศาสตร์ของหอกลั่นไอน้ำแบบเปิด เพื่อนำมาใช้หาปริมาณอัตราส่วนที่เหมาะสมในการป้อนกลับของของเหลวผลิตภัณฑ์ที่ได้หลังจากการกลั่นเข้าสู่หอกลั่น ในกรณีที่ต้องการออกแบบให้หอกลั่นมีขนาดเล็กที่สุด (จำนวนชั้นของหอกลั่นน้อยที่สุด) ซึ่งในเบื้องต้นนั่นคาดว่าจะสามารถสร้างสมการที่สามารถแก้ได้โดยง่าย แต่เมื่อสร้างสมการขึ้นมาสำเร็จ สมการที่ได้นั้นมีความซับซ้อนมาก จนไม่สามารถแก้โดยใช้ระบบวิธีการทางการวิเคราะห์ได้ อย่างไรก็ตามสมการที่ถูกสร้างขึ้นนี้สามารถแก้ได้โดยใช้ระบบวิธีการทางตัวเลขในทุก ๆ สภาวะการทดลอง ซึ่งในรายงานนี้ก็ได้แสดงตัวอย่างการแก้สมการไว้ด้วย

Abstracts

The program is assembled from four research projects of modeling physical phenomena in applied sciences. These projects are connected by the methods applied in mathematical physics, mathematical analysis of differential equations used for modeling.

The research performed in the first project can be formally separated in three parts. All these parts are related by the method of the study and the sequence of discoveries. The first part of the project deals with modeling in fluid dynamics. A systematic application of the group analysis method for modeling fluids with internal inertia is presented. The group classification separates these models into 73 different classes. The second part of the project deals with applications of the group analysis method to integro-differential equations. The research deals with an evolutionary integro-differential equation describing nonlinear waves. We discuss new approaches developed in modern group analysis and apply them to the general model considered in the present paper. Reduced equations and exact solutions are also presented. Another application of the group analysis method to integro-differential equations is related with the Boltzmann equation. The group classification with respect to sources is carried out for the equations under consideration using the algebraic method. The third part of the first project is focused on the study of two problems: (a) on first integrals of second-order ordinary differential equations; (b) the complete group classification of systems of two linear second-order ordinary differential equations with constant coefficients. Here we discuss first integrals of a particular representation associated with second-order ordinary differential equations. The relationship between the integral form, the associated equations, equivalence transformations, and some examples are considered as part of the discussion illustrating some important aspects and properties. For group classification the present project corrects the way of using Jordan canonical forms for studying the symmetry structures of systems of linear second-order ordinary differential equations with constant coefficients applied in (Wafo Soh (2010)). The approach is demonstrated for a system consisting of two equations.

In the second research the problem of a two-dimensional fully mixed region collapsing in continuously density-stratified medium is considered. This research deals with the numerical treatment of the advective terms in the Navier-Stokes equations in the Oberbeck-Bousinesq approximation. Comparisons are made between the upwind scheme, flux-limiter schemes namely Minmod, Superbee, Van Leer and Monotonized Centred (MC), monotone adaptive stencil schemes namely ENO3 and SMIF, and weighted stencil scheme WENO5. Laboratory experimental data of Wu (J. Fluid Mech. , 1969, vol. 35) are used as a benchmark test to compare performance of different numerical approaches. We found that flux limiter schemes have smallest numerical diffusion. The WENO5 scheme describes more accurately the width of collapse region variation with time. All considered schemes give realistic patterns of internal gravity waves generatrd by collapse region.

In the third research a variational model for the reduction of speckle noise in ultrasound images is developed, which assumes that speckle noise follows a Rayleigh distribution. The model leads to a functional on the space of functions of bounded

variation to be minimized. This functional consists of an energy term and a data-fidelity term derived from the Rayleigh distribution. It is shown that minimizers of the functional exist and, under some additional assumptions, are unique. The solution of the resulting Euler-Lagrange equation is then approximated by the gradient descent method. For the purpose of verification of the model, a pattern image as well as the Lenna image are used as sample images, and the correlations between the noisy, respectively the reconstructed images and the original ones are compared. It is found that the model can be used successfully to remove noise from images and ultrasound videos. Finally, the performance of this new model is compared with that of some of the variational denoising models described in the literature, by means of the sample images.

The fourth research study has successfully produced a mathematical model that can be used to predict the rate of solution mediated transformation of polymorphs and also aid understanding of the phenomenon. The model results have been compared with experimental values of the solution mediated transformation of α-DL-methionine into γ-DL-methionine (time dependent methionine concentration and polymorph mass fraction results). Initially the parameters in the model were fitted based on experimental measurements of crystal growth kinetics, nucleation kinetics, dissolution kinetics and induction times for the two polymorphs; there were no parameters in the model that were fitted using solution mediated transformation data. This model showed the same trends as the experimental data, but the rate of transformation was not correct. Analysis of the results showed that the only parameter that could be responsible for the mismatch was the dissolution rate constant; when this result was fitted based on solution mediated transformation results then the fit was very good. Reasons for the mismatch are also discussed. A second study was made of modeling open steam distillation columns in order to solve for the reflux ratio resulting in a minimum number of stages. It was hoped to be able to find an analytical solution to the problem, however while an equation could be found that gave the solution, the equation was very complex and could not be analytically solved. The equation could be solved numerically for any set of operating conditions, and example solutions are shown in this report.

Contents

Chapter 1

Analytical study of differential equations with applications

1.1 Introduction

Many important physical processes in nature are governed by partial differential equations (PDEs). For this reason, the knowledge of the mathematical character and properties of the governing equations are required. Properties of PDEs can be effectively studied by using their exact solutions. Therefore, there is interest in finding exact solutions of PDEs. In general, it is not easy to obtain exact solutions of PDEs. One of the methods for obtaining exact solutions is the group analysis method. It is well-known that the group analysis method is a powerful and direct approach to construct exact solutions of PDEs.

The research performed in the project can be formally separated in three parts. All these parts are related by the method of the study and the sequence of discoveries.

1.1.1 Fluids with internal inertia

The first part of the project deals with modeling in fluid dynamics.

Developing new technology requires developing new models in fluid dynamics. Equations of fluids with internal inertia is the new theory considered in the fluid dynamics. These equations are obtained on the basis of the Euler-Lagrange principle. Among fluids with internal inertia there are two intensively studied classes of models. This project is focused on group classification of a class of dispersive models [1][1]

$$\begin{gathered}\dot{\rho}+\rho\, div(u)=0, \quad \rho\dot{u}+\nabla p=0, \quad \dot{S}=0,\\ p=\rho\tfrac{\delta W}{\delta\rho}-W=\rho(\tfrac{\partial W}{\partial\rho}-\tfrac{\partial}{\partial t}(\tfrac{\partial W}{\partial\dot{\rho}})-div(\tfrac{\partial W}{\partial\dot{\rho}}u))-W,\end{gathered} \tag{1.1}$$

where t is time, ∇ is the gradient operator with respect to space variables, ρ is the fluid density, u is the velocity field, $W(\rho,\dot{\rho},S)$ is a given potential, 'dot' denotes the material time derivative: $\dot{f}=\frac{df}{dt}=f_t+u\nabla f$ and $\frac{\delta W}{\delta\rho}$ denotes the variational derivative of W with respect to ρ at a fixed value of u. These models include the non-linear one-velocity model of a bubbly fluid (with incompressible liquid phase) at small volume concentration of gas bubbles (Iordanski (1960) [2], Kogarko (1961) [3],Wijngaarden (1968) [4]), and the dispersive shallow water model (Green & Naghdi (1975) [5], Salmon (1998) [6]). Equations (1.1) were obtained in [1] using the Lagrangian of the form

$$L=\frac{1}{2}|u|^2-W(\rho,\dot{\rho},S).$$

[1]See also references therein.

This is an example of a medium behavior dependent not only on thermodynamical variables but also on their derivatives with respect to space and time. In this particular case the potential function depends on the total derivative of the density which reflects the dependence of the medium on its inertia.

A complete group classification of equations (1.1), where $W = W(\rho, \dot{\rho})$ is performed in [7] (one-dimensional case) and [8] (three-dimensional case). Invariant solutions of some particular cases which are separated out by the group classification are considered in [7, 8, 9]. Group classification of the class of models describing the behavior of a dispersive continuum with $\varepsilon = \varepsilon(\rho, |\nabla\rho|)$ was studied in [10]. It is also worth to notice that the classical gas dynamics model corresponds to $W = W(\rho, S)$ (or $\varepsilon = \varepsilon(\rho, S)$). A complete group classification of the gas dynamics equations was presented in [11]. Later, an exhausting program of studying the models appearing in the group classification of the gas dynamics equations was announced in [12]. Some results of this program were summarized in [13].

1.1.2 Application of the group analysis method to integro-differential equations

The second part of the project deals with applications of the group analysis method to integro-differential equations.

In applied mathematics and physics special attention is given to the study of invariant solutions of integro-differential equations which are directly associated with fundamental symmetry properties of these equations. Group analysis in this case is a universal tool for obtaining complete sets of symmetries. However a direct transference of the known scheme of the group analysis method on integro-differential equations is impossible. A general algorithm for application of the group analysis to equations with nonlocal terms was proposed recently [14]. It is worth to notice that this area of the group analysis method is still developing. In the present research the group analysis method is applied to two integro-differential equations: (a) the Rudenko equation, and (b) the Boltzmann equation with sources.

The Rudenko equation

One of the most general evolution equations used in nonlinear wave physics is the following one [15, 16]:

$$\begin{array}{l} \left(u_x - uu_t - w_{tt}\right)_t = u_{yy} + u_{zz}\,, \\ w = \int_0^\infty K\left(s\right)\, u\left(t-s\right) ds \end{array} \,. \tag{1.2}$$

Here the variable t is the time, and x, y, z are the spatial Cartesian coordinates. The coordinate x is distinguished as a "longitudinal" one. It coincides with a preferred orientation of the wave propagation. The other coordinates y, z are identified as "transversal" ones. They are commonly introduced in the cross-section of a wave beam.

Special cases of the equation (1.2) are well-known. In particular, if the kernel is identically zero, $K\left(s\right) \equiv 0$, the general equation (1.2) is reduced to the Khokhlov-Zabolotskaya (KZ) equation [17, 18], describing wave beams in nonlinear media:

$$\left(u_x - uu_t\right)_t = u_{yy} + u_{zz}. \tag{1.3}$$

If the kernel is the delta-function, $K = 2\delta\left(s\right)$, the model (1.2) leads to the equation

$$\left(u_x - uu_t - u_{tt}\right)_t = u_{yy} + u_{zz} \tag{1.4}$$

for nonlinear beams in a dissipative medium [19, 20]. Equation (1.4) is known as the Khokhlov-Zabolotskaya-Kuznetsov (KZK) equation. It is widely used in underwater acoustics for engineering design of parametric radiating and receiving arrays [20].

If the kernel is proportional to the derivative of the delta-function, $K = 2\delta'(s)$, the integro-differential equation (1.2) becomes the Kadomtsev-Petviashvili (KP) equation

$$(u_x - uu_t - u_{ttt})_t = u_{yy} + u_{zz} \tag{1.5}$$

for nonlinear beams in a dispersive medium [21, 22]. The similar equation

$$(u_x - uu_t - u_{tttt})_t = u_{yy} + u_{zz} \tag{1.6}$$

for a scattering medium [23] follows from (1.2) when $K = 2\delta''(s)$.

There exist other models that specify or generalize the equation (1.2), e.g. by including (1.2) in a coupled systems of nonlinear equations [24, 25].

In the present research we apply our method [26, 27] to the Rudenko equation.

The Boltzmann equation with sources

The Boltzmann kinetic equation is the basis of the classical kinetic theory of rarefied gases. Considerable interest in the study of the Boltzmann equation was always the search for exact (invariant) solutions directly associated with the fundamental properties of the equation. After the studies of the class of the local Maxwellians [28, 29, 30] new classes of invariant solutions were constructed in the 1960s in [31, 32, 33]. A decade later the BKW-solution was almost simultaneously derived in [34] and in [35]. Contrary to the Maxwellians, the Boltzmann collision integral does not vanish for this solution. The discovery of the BKW-solution stimulated a great splash of studies of exact solutions of various kinetic equations. However, the progress at that time was really limited to the construction of BKW-type solutions for different simplified models of the Boltzmann equation [36].

The Boltzmann equation is an integro-differential equation. Whereas the classical group analysis method has been developed for studying partial differential equations, the main obstacle for applying group analysis to integro-differential equations comes from presence of nonlocal integral operators. The direct group analysis for equations with nonlocal operators was worked out and successfully used in [26, 37, 14]. In particular, a complete group classification of the spatially homogeneous and isotropic Boltzmann equation without sources was obtained in [26, 27].

In the present research we use our method [26, 27] to amend the results of [38]. A group classification of the equation for a moment generating function with respect to a source function is obtained.

1.1.3 Application of group analysis to ordinary differential equations

Many methods of solving differential equations use a change of variables that transform a given differential equation into another equation with known properties. Since the class of linear equations is considered to be the simplest class of equations, it was attractive to transform a given differential equation into a linear equation. This problem, which is called a linearization problem, is a particular case of the equivalence problem. The equivalence problem can be formulated as follows. Let a set of invertible transformations

be given. One can introduce the equivalence property according to these transformations: two differential equations are equivalent if there is a transformation of the given set which transforms one equation into another. The equivalence problem involves a number of related problems such as defining a class of transformations, finding invariants of these transformations, obtaining the equivalence criteria, and constructing the transformation.

The third part of the present project is focused on the study of two problems: (a) on first integrals of second-order ordinary differential equations; (b) the complete group classification of systems of two linear second-order ordinary differential equations with constant coefficients.

First integrals of second-order ordinary differential equations

We give a short review of results related with an equivalence problem for a second-order ordinary differential equation. Two types of transformations can be distinguished among the transformations used in the equivalence problem for second-order ordinary differential equations: point transformations and the generalized Sundman transformations. S.Lie [39] also noted that all second-order ODEs can be transformed to each other by means of contact transformations, thus this set of transformations cannot be applied for a classification of second-order ODEs.

The researches of the linearization problem motivated us to study equations possessing a first integral of the form

$$I = \frac{\dot{x}\tilde{A}(t,x) + \tilde{C}(t,x)}{\dot{x}\tilde{B}(t,x) + \tilde{Q}(t,x)}. \tag{1.7}$$

Notice that a second-order equation equivalent to the free particle equation via the generalized Sundman transformation also possesses a first integral of the form (1.7).

The authors of [40, 41, 42] came to the form of first integral (1.7) from the study of λ-symmetries for second-order equations which play a fundamental role. Although the equation may lack Lie point symmetries, there always exists a λ-symmetry associated to a first integral $I = I(t, x, \dot{x})$.

Group classification of systems of two linear second-order ordinary differential equations with constant coefficients

Recent works by C.Wafo Soh [43] have focused on the study of systems of second-order ordinary differential equations with constant coefficients. The studies deal with symmetries of systems of linear second-order ordinary differential equations with two and three equations are considered. The goal of the present research is to study the symmetry structure of a system of n, $(n = 2, 3)$ linear second-order ordinary differential equations with constant coefficients. Since a change of the dependent and independent variables does not change the structure of the admitted Lie group, the author at first simplify the system, and then calculate the admitted Lie group of the simplified system using the standard procedure.

The goal of the present research is to correct the approach applied in [43]. The approach is illustrated by using a complete study of symmetry structures of systems of two real-valued linear second-order ordinary differential equations with constant coefficients. In application of this approach to a system with more than two equations one needs to take into account that if a real-valued matrix M has a complex eigenvalue, then the conjugate number is also an eigenvalue. Only systems of two second-order equations are considered here.

1.2 Summary of the main results

The outcomes of this research are 5 papers in International journals and 1 paper in Proceedings of International conference with peer reviewing.

1.2.1 Fluids with internal inertia

A systematic application of the group analysis method for modeling fluids with internal inertia is considered in this part of the research. The equations studied include models such as the nonlinear one-velocity model of a bubbly fluid (with incompressible liquid phase) at small volume concentration of gas bubbles, and the dispersive shallow water model. These models are obtained for special types of the potential function $W(\rho, \dot{\rho}, S)$. The main feature of the present research is the study of the potential functions with $W_{\dot{\rho}\dot{\rho}S} \neq 0$. The group classification separates these models into 73 different classes. The result is published in [44].

1.2.2 Applications of group analysis to integro-differential equations

The Rudenko equation

The research deals with an evolutionary integro-differential equation describing nonlinear waves. A particular choice of the kernel in the integral leads to well-known equations such as the Khokhlov-Zabolotskaya equation, the Kadomtsev-Petviashvili equation and others. Since the solutions of these equations describe many physical phenomena, the analysis of the general model studied in this paper is important. One of the methods for obtaining solutions of differential equations is provided by the Lie group analysis. However, this method is not applicable to integro-differential equations. Therefore, in the research we discuss new approaches developed in modern group analysis and apply them to the general model considered in this paper. Reduced equations and exact solutions are also presented. The result is published in [45].

The Boltzmann equation with sources

This part of the research considered in the project is started after visiting Suranaree University of Technology by Professor Yu.N.Grigoriev. We started with the following problem. In [38] the classical group analysis method was applied to the equation which was obtained from the spatially homogeneous and isotropic Boltzmann equation with sources. The derived equation is still a nonlocal partial differential equation. However, this property was not taken into account there. In the present paper this lack of [38] is corrected. The result is published in [46, 47].

1.2.3 Application of group analysis to ordinary differential equations

On first integrals of second-order ordinary differential equations

This part of the research considered in the project is devoted to the study of intermediate integrals of a second-order ordinary differential equation of the form

$$I = \frac{\dot{x}A(t,x) + C(t,x)}{\dot{x}B(t,x) + Q(t,x)}.$$

This research is started after visiting Suranaree University of Technology by Professor Sibusiso Moyo (DUT, South Africa). The sufficient conditions for existence of an intermediate integral of the form presented above are obtained. The result is published in [48].

Complete group classification of systems of two linear second-order ordinary differential equations with constant coefficients

Recent works by Wafo Soh [43] have focused on the study of systems of second-order ordinary differential equations with constant coefficients. The studies deal with symmetries of systems of linear second-order ordinary differential equations with two and three equations are considered. The research conducted in the project corrects the way of using Jordan canonical forms for studying the symmetry structures of systems of linear second-order ordinary differential equations with constant coefficients applied by Wafo Soh. The result is published in [49].

1.3 Acknowledgements

The research was supported by Suranaree University of Technology and by the Office of the Higher Education Commission under the NRU project.

Bibliography

[1] S. L. Gavrilyuk and V. M. Teshukov. Generalized vorticity for bubbly liquid and dispersive shallow water equations. *Continuum Mech. Thermodyn.*, 13:365–382, 2001.

[2] S. V. Iordanski. On the equations of motion of the liquid containing gas bubbles. *Zhurnal Prikladnoj Mekhaniki i Tekhnitheskoj Fiziki*, (3):102–111, 1960.

[3] B. S. Kogarko. On the model of cavitating liquid. *Dokl. AS USSR*, 137:1331–1333, 1961.

[4] van L. Wijngaarden. On the equations of motion for mixtures of liquid and gas bubbles. *J. Fluid Mech.*, 33:465–474, 1968.

[5] A. E. Green and P. M. Naghdi. A derivation of equations for wave propagation in water of variable depth. *J. Fluid Mech.*, 78:237–246, 1976.

[6] R. Salmon. *Lectures on Geophysical Fluid Dynamics*. Oxford University Press, New York, 1998.

[7] A. Hematulin, S. V. Meleshko, and S. G. Gavrilyuk. Group classification of one-dimensional equations of fluids with internal inertia. *Mathematical Methods in the Applied Sciences*, 30:2101–2120, 2007.

[8] P. Siriwat and S. V. Meleshko. Applications of group analysis to the three-dimensional equations of fluids with internal inertia. *Symmetry, Integrability and Geometry: Methods and Applications (SIGMA)*, 4(027):1–19, 2008.

[9] A. Hematulin and P. Siriwat. Invariant solutions of the special model of fluids with internal inertia. *Communications in Nonlinear Science and Numerical Simulation*, 14:2111–2119, 2009.

[10] P. Voraka and S. V. Meleshko. Group classification of one-dimensional equations of fluids with internal energy depending on the density and the gradient of the density. *Continuum Mech. Thermodyn.*, 20:397–410, 2009.

[11] L. V. Ovsiannikov. *Group analysis of differential equations*. Nauka, Moscow, 1978. English translation, Ames, W.F., Ed., published by Academic Press, New York, 1982.

[12] L. V. Ovsiannikov. Program SUBMODELS. Gas dynamics. *J. Appl. Maths Mechs*, 58(4):30–55, 1994.

[13] L. V. Ovsiannikov. Some results of the implementation of the "PODMODELI" program for the gas dynamics equations. *J.Appl. Maths Mechs*, 63(3):349–358, 1999.

[14] Yu. N. Grigoriev, N. H. Ibragimov, V. F. Kovalev, and S. V. Meleshko. *Symmetries of integro-differential equations and their applications in mechanics and plasma physics.* Lecture Notes in Physics, Vol. 806. Springer, Berlin / Heidelberg, 2010.

[15] O. V. Rudenko and S. I. Soluyan. *Theoretical Foundations of Nonlinear Acoustics.* Plenum, Consultants Bureau, New York, 1977.

[16] O. V. Rudenko, S. I. Soluyan, and R. V. Khokhlov. Problems of the theory of nonlinear acoustics. *Sov. Phys. Acoustics*, 20(3):356–359, 1974.

[17] E. A. Zabolotskaya and R. V. Khokhlov. Quasi-plane waves in the nonlinear acoustics of confined beams. *Sov. Phys. Acoustics*, 15(1):35–40, 1969.

[18] O. V. Rudenko. The 40th anniversary of the Khokhlov-Zabolotskaya equation. *Acoustical Physics*, 56(4):457–466, 2010.

[19] V. P. Kuznetsov. Equations of nonlinear acoustics. *Sov. Phys. Acoustics*, 16(4):548–553, 1970.

[20] B. K. Novikov, O. V. Rudenko, and V. I. Timoshenko. *Nonlinear Underwater Acoustics.* American Inst. of Physics, New York, 1987.

[21] B. B. Kadomtsev and V. I. Petviashvili. On the stability of solitary waves in weakly dispersive media. *Sov. Phys. Doklady*, 15:539–541, 1970.

[22] U. A. Danilov. Kadomtsev-Petviashvili equation. In *Enceklopedia of Physics*, page 229. Soviet Enceklopedia, Moscow, 1990.

[23] O. V. Rudenko and V. A. Robsman. Equation of nonlinear waves in a scattering medium. *Doklady Physics*, 47(6):443–446, 2002.

[24] O. V. Rudenko. Nonlinear sawtooth-shaped waves. *Physics-Uspekhi (Advances in Physical Sciences)*, 38(9):965–989, 1995.

[25] O. V. Rudenko and O. A. Sapozhnikov. Self-action effects for wave beams containing shock fronts. *Physics-Uspekhi (Advances in Physical Sciences)*, 47(9):907–922, 2004.

[26] Yu. N. Grigoriev and S. V. Meleshko. Investigation of invariant solutions of the Boltzmann kinetic equation and its models, 1986. Preprint of Institute of Theoretical and Applied Mechanics.

[27] Yu. N. Grigoriev and S. V. Meleshko. Group analysis of the integro–differential Boltzman equation. *Dokl. AS USSR*, 297(2):323–327, 1987.

[28] J. C. Maxwell. On the dynamical theory of gases. *Philosophical Transactions of the Royal Society of London*, 157:49 – 88, 1867.

[29] L. Boltzmann. Further studies on the thermal equilibrium among gas-molecules (Weitere Studien über das Wärmegleichgewicht unter Gasmolekülen). *Sitzungsberichte der Akademie der Wissenschaften, Mathematische-Naturwissenschaftliche Klasse*, 66:275 – 370, 1872.

[30] T. Carleman. *Problemes Mathematiques Dans la Theorie Cinetique des Gas*, volume 2. Publications Scientifiques de l'Institut Mittag-Leffler, Uppsala, 1957.

[31] A. A. Nikolskii. The simplest exact solutions of the Boltzmann equation of a rarefied gas motion. *Dokl. AS USSR*, 151(2):299–301, 1963.

[32] A. A. Nikolskii. Three dimensional homogeneous expansion–contraction of a rarefied gas with power interaction functions. *Dokl. AS USSR*, 151(3):522–524, 1963.

[33] A. A. Nikolskii. Homogeneous motion of displacement of monatomic rarefied gas. *Inzhenerny journal*, 5(4):752–755, 1965.

[34] A. V. Bobylev. On exact solutions of the Boltzmann equation. *Dokl. AS USSR*, 225(6):1296–1299, 1975.

[35] M. Krook and T. T. Wu. Formation of Maxwellian tails. *Phys. Rev. Lett.*, 36(19):1107–1109, 1976.

[36] M. H. Ernst. Nonlinear model–Boltzmann equations and exact solutions. *Phys. Rep.*, 78:1–171, 1981.

[37] S. V. Meleshko. *Methods for Constructing Exact Solutions of Partial Differential Equations*. Mathematical and Analytical Techniques with Applications to Engineering. Springer, New York, 2005.

[38] T. F. Nonenmacher. Application of the similarity method to the nonlinear Boltzmann equation. *J. of Appl. Mathem. and Physics (ZAMP)*, 35(5):680–691, 1984.

[39] S. Lie. Klassifikation und Integration von gewöhnlichen Differentialgleichungen zwischen x, y, die eine Gruppe von Transformationen gestatten. III. *Archiv for Matematik og Naturvidenskab*, 8(4):371–427, 1883. Reprinted in Lie's Gessammelte Abhandlungen, 1924, 5, paper XIY, pp. 362–427.

[40] C. Muriel and J. L. Romero. Integrating factors and $\lambda-$symmetries. *Journal of Nonlinear Mathematical Physics*, 15:290–299, 2008.

[41] C. Muriel and J. L. Romero. First integrals, integrating factors and λ-symmetries of second-order differential equations. *J. Phys. A: Math. Theor.*, 42(365207):17pp, 2009.

[42] C. Muriel and J. L. Romero. Second-order ordinary differential equations and first integrals of the form $a(t, x)\dot{x} + b(t, x)$. *Journal of Nonlinear Mathematical Physics*, 16:209–222, 2009.

[43] C. Wafo Soh. Symmetry breaking of systems of linear second-order differential equations with constant coefficients. *Communications in Nonlinear Science and Numerical Simulations*, 15:139–143, 2010.

[44] P. Siriwat and S. V. Meleshko. Group classification of one-dimensional nonisentropic equations of fluids with internal inertia. *Continuum Mech. Thermodyn.*, 24:115–148, 2012.

[45] N. H. Ibragimov, S. V. Meleshko, and O. V. Rudenko. Group analysis of evolutionary integro-differential equations describing nonlinear waves: General model. *Journal of Phys. A: Mathematical and Theoretical*, 44(315201), 2011.

[46] Yu. N.Grigoriev and S. V. Meleshko. On group classification of the spatially homogeneous and isotropic Boltzmann equation with sources. *International Journal of Non-Linear Mechanics*, 47:1014–1019, 2012.

[47] Yu. N.Grigoriev, S. V. Meleshko, and A. Suriyawichitseranee. On the equation for the power moment generating function of the Boltzmann equation. group classification with respect to a source function. In O.O. Vaneeva, C. Sophocleous, R.O. Popovych, P.G.L. Leach, V.M. Boyko, and P.A. Damianou, editors, *Group Analysis of Differential Equations & Integrable Systems*, pages 98–110. University of Cyprus, Nicosia, 2013.

[48] S. V. Meleshko, S. Moyo, C. Muriel, J. L. Romero, P. Guha, and A.G.Choudhury. On first integrals of second-order ordinary differential equations. *Journal of Engineering Mathematics*, 82:17–30, 2013. DOI 10.1007/s10665-012-9590-9.

[49] S. V. Meleshko. Comment on "Symetry breaking of systems of linear second-order ordinary differential equations with constant coefficients". *Communications in Nonlinear Science and Numerical Simulations*, 16:3447–3450, 2011.

Chapter 2

Mathematical modeling in fluid dynamics: numerical and analytical solutions of the Navier-Stokes equations

2.1 Introduction

A flow generated by local density perturbation (mixed region) in stratified medium is considered. The interest to the problem stems from the study of a number of geophysical phenomenon and a number of technical problems. For example, because the turbulent wake behind a body traveling through stratified fluid is very slender in the direction of body motion, the induced by wake flow field and internal waves can be adequately described by studding collapse of non-turbulent mixed region in stratified medium. There are numerous studies focusing on locally homogeneous perturbation of density the field (fully mixed region). Experimental work has been done in this problem by Wu [1].This problem was used by several researchers as a benchmark test in order to assess the performance of constructed numerical algorithms. Analysis of the known literature on numerical modeling of flow generated by collapse of mixed region in a linearly stratified medium shows that there are no studies on applicability of high-order resolution advection finite-difference schemes to this problem with discontinuity in the density field.

The variable density incompressible viscous flow presents the difficulty of satisfying the property of mass conservation in two respects. On the one hand, the mass density of each fluid particle must remain unchanged during the fluid motion, whatever the level of unsteadiness and mixing. On the other hand, the velocity field must satisfy the incompressibility constraint which reflects the inability of pressure to do compression work. These two important physical characteristics are fully described by the set of the incompressible Navier-Stokes equations augmented by the advection equation for the density. The sharp front discontinuities are transported from one location to another, described very well by an advection model. The problem of accurately modeling advection is not limited to the area of geophysical models. In regions with large substance gradients and/or velocities the advection scheme that is used in many models (upwind-first order, central differences-second order) leads to significant diffusion and/or under and overshoot of substance values. To describe accurately enough the sharp discontinuity in density at the mixed region edge, the schemes of high order of approximation are

required. Godunov's theorem states that any linear monotonic advection scheme can not provide more than first-order accuracy. Therefore, there is a need to apply higher order accuracy numerical schemes devised for numerical solutions of conservation laws which support discontinuous solutions. Computational experience demonstrates that numerical solutions better reproduce the physical phenomenon, if they satisfy additional properties such as conservativeness, monotonicity, maximum principle, total variation diminishing and others. Many methods match additional requirements, they are, for example, Lax-Wendroff, Lax-Friedrichs, flux corrected transport (FCT) methods of Boris-Book and Zalesak, slope limiter methods of Van Leer, essentially non-oscillatory (ENO) schemes of Harten-Shu-Osher and total variation diminishing schemes (TVD). Even though there are very little theoretical results about properties of such schemes in multidimensional and non linear cases, in practice these schemes are very robust, and stable, and are used in a lot of practical applications. Nevertheless, there is always the question of what is the best choice, which usually is problem dependent. In this research several high order resolution advection schemes are used to solve the problem of mixed region dynamics in a stratified fluid. A comparative analysis of the effectiveness of the advection schemes was obtained.

2.2 Summary of the main results

The governing equations are the Navier-Stokes equations in the Oberbeck-Boussinesq approximation. To study the shape of mixed region, the historic idea of nondiffusing passive scalar will be used. The transport equation of passive scalar is solved together with the system of Navier-Stokes. A finite difference scheme is used to simulate the governing equations. Variables are discretized on a uniform rectangular grid. The fractional time-stepping, Chorin-Temams idea is used for solving incompressible Navier-Stokes equations. To solve the advection equation the explicit high-resolution monotone algorithm is used. A Crank-Nikolson discretizating was utilized for the diffusion part of the equation. To describe accurate enough the discontinuity in density at mixed region edge the monotone scheme of high order of approximation is required. The different numerical approximations of the advection term used in our work are presented by four flux-limiter methods, two adaptive stencil methods, and one weighted stencil method. Flux-limiter schemes satisfy many of the requirements of a good advection scheme. In particular they are Total Variation Diminishing (TVD), mass conservative and less diffusive than the simpler schemes. The idea behind the adaptive stencil methods is to keep the total number of cells in the stencil constant, and to change the left shift w of the stencil if necessary with the spatial coordinate in order to avoid including the cell with the discontinuity in the interpolating polynomial. The adaptive stencil method used in this work is a hybrid monotonic difference scheme developed by Gushchin and Belotserkovskii for the numerical simulation of fluid flows with large gradients of hydrodynamic parameters. The Splitting on physical factors Method for Incompressible Fluid flows (SMIF) is based on a combination of a Modified Central Difference Scheme MCDS and Modified Upwind Difference Scheme MUDS with special switch condition. The splitting scheme is similar to the famous SMAC method Amsden and Harlow and to one of the approaches suggested in Fortin.The second adaptive stencil method used in this work is the third order essentially non oscillatory (ENO3) scheme.

The WENO scheme is a weighted stencil method in which the idea is once again to define a number of candidate stencils at each grid location, but instead of selecting one of them for calculating the numerical flux, a convex combination of all candidate stencils

is used. Finite difference WENO5 scheme uses the same sense of applying ENO3 to construct cell faces numerical fluxes. But WENO5 uses a combination of 3 stencils for construction interpolate polynomials depending on upwinding.

The comparative study has shown that among flux-limiter schemes the Superbee limiter gives the better results concerning value of the numerical diffusion and as well, Superbee flux limiter gives smallest numerical diffusion compared with SMIF, ENO3 and WENO5 schemes. Performance of ENO3 and SMIF were nearly identical. WENO5 produces smaller smearing of discontinuity compared with ENO3 and SMIF schemes. Superbee limiter gives width of mixed region a little bit smaller compared with Wu's experimental data. WENO5 scheme demonstrates closer results with Wu's experimental data. More significant, influence of different high-order upwind approximations on the patterns of internal waves generated are observed for the waves with density level corresponding to the density of unperturbed fluid on the levels of mixed region.

The results are published in [2].

2.3 Acknowledgements

The research was supported by Suranaree University of Technology and by the Office of the Higher Education Commission under the NRU project.

Bibliography

[1] J. Wu. Mixed region collapse with internal wave generation in a density-stratified medium. *J. Fluid. Mech.*, 35(3):531, 1969.

[2] N. P. Moshkin, G. G. Chernykh, and Kridsada Narong. On the performance of high resolution non-oscillating advection schemes in the context of the flow generated by a mixed region in a stratified fluid. *Mathematics and Computers in Simulation*, 127:203–219, 2016.

Chapter 3

Ultrasound image enhancement by means of a variational approach

3.1 Introduction

Image noise is present in practically all kinds of imaging, whether analog or digital. Consequently, image noise reduction is a very active and intense field of research. The type of noise most noticeable in ultrasound images is speckle noise, which appears in an image as very dark or very bright spots. It results in reduced image quality by blurring fine details such as edges, shapes, pixel intensity values etc.

Many popular denoising techniques involve local averaging, by considering the local statistics of the image. The best known include the Lee filter [7], the Frost filter [4] and the Kuan filter [5]. Over time there have been numerous refinements to these filters in order to improve their performance. Another set of noise reduction techniques is global in nature, the most common of which are thresholding methods and variational methods. Among the tresholding methods, wavelet methods [2,3] have seen widespread interest.

In the variational method popularized by the paper of Rudin, Osher and Fatemi [8], the denoising problem is formulated as an optimization problem: The denoised image u is obtained as the minimizer of a functional

$$E(u) = \beta \iint_\Omega |\nabla u| \, dA \; + \; \iint_\Omega J(u, f) \, dA, \tag{1}$$

where ∇u denotes the gradient, f the noisy image and $J(u, f)$ is a data-fidelity term. The first integral involving the gradient results in smoothing of the image, while the second integral involving the data fidelity term measures how well the denoised image matches the noisy image. The parameter β specifies how the two components of this functional are weighed against another in this functional. By the method of calculus of variations, the minimizer u can be found numerically as the solution of an Euler-Lagrange equation

$$\frac{\partial}{\partial x}\left(\frac{u_x}{u_x^2 + u_y^2}\right) + \frac{\partial}{\partial y}\left(\frac{u_y}{u_x^2 + u_y^2}\right) - \frac{1}{\beta}\frac{\partial}{\partial u} J(u, f) = 0,$$

where the outward normal vanishes on the boundary of the image region Ω. In the original paper [8], the second integral in (1) was simply chosen to represent the mean square error. It is, however, natural to assume that this integral should depend on the characteristics noise. Le, Chatrand and Asaki [6], using Bayesian statistics, derived a data fidelity term $J(u, f)$ for radiography images by assuming that noisy pixel intensity

has the Poisson distribution. On the other hand, in ultrasound imaging the noisy image pixel intensity is generally modeled to have the Rayleigh distribution [1]. This research thus derives the data fidelity term which appropriate for the Rayleigh distribution. In addition, mathematical results on the existence and uniqueness of solutions to variational problem (1) given our fidelity term are proved.

3.2 Summary of the main results

In detail, the following results were achieved:

1. *Derivation of the data-fidelity term.* Using Bayesian statistics, the data fidelity term appropriate for the Rayleigh distribution was obtained in the form of

$$J(u, f) = 2 \ln u + \frac{f^2}{u^2}. \tag{2}$$

2. *Theoretical considerations.* The following assumptions had to be imposed:

   (A1) Ω is a bounded, open subset of $\mathbb{R}^2$ with Lipschitz boundary,

   (A2) Let $S(\Omega)$ denote the set of functions defined on Ω which are positive a.e. and of bounded variation. The denoised image u is sought in the class $S(\Omega)$.

   (A3) The noisy image f is essentially bounded and is essentially bounded below away from zero, i.e. there exist real numbers m and M so that $0 < m \leq f(\omega) \leq M$ a.e.

   We also set $Q(\Omega) = \{\, u \in S(\Omega) \,:\, u(w) \leq \sqrt{3} f(\omega) \text{ a.e.} \,\}$.

   The following theorems were proved, assuming data fidelity term (2):

   Theorem 7: (Existence of minimizers) *Let Ω and f satisfy properties (A1) and (A3), respectively. Then there exists $\hat{u} \in S(\Omega)$ satisfying*

   (a) $m \leq \hat{u}(\omega) \leq M$ a.e. $\omega \in \Omega$.

   (b) $E(\hat{u}) \leq E(u)$ for all $u \in S(\Omega)$.

   Theorem 8: (Mild uniqueness of minimizers) *Let Ω and f satisfy properties (A1) and (A3), respectively. Then there exists at most one $\hat{u} \in Q(\Omega)$ satisfying $E(\hat{u}) \leq E(u)$ for all $u \in S(\Omega)$.*

   Corollary 9: (Uniqueness of minimizers) *Let Ω and f satisfy properties (A1) and (A3), respectively. Then there exists a unique $\hat{u} \in Q(\Omega)$ satisfying $E(\hat{u}) \leq E(u)$ for all $u \in Q(\Omega)$. Furthermore, $m \leq \hat{u}(\omega) \leq M$ a.e. $\omega \in \Omega$.*

   Theorem 10: (Monotonicity of minimers) *Let f_1 and f_2 satisfy property (A3) with $f_1 \leq f_2$, and let u_1 and u_2 denote minimizers of E on Ω corresponding to f_1 and f_2, respectively. Set $A = \{\, \omega \in \Omega : f_1(\omega) < f_2(\omega) \,\}$. Then $u_1(\omega) \leq u_2(\omega)$ a.e. $\omega \in A$. In particular, if $f_1(\omega) < f_2(\omega)$ a.e., then $u_1(\omega) \leq u_2(\omega)$ a.e.*

3. *Numerical simulations* on some standard images with noise imposed were performed using Matlab. The simulations show that our method can effectively denoise images, and is as good or slightly better performant than other variational methods.

3.3 Acknowledgements

This research was supported by Suranaree University of Technology and by the Office of the Higher Education Comission under the NRU project.

Bibliography

[1] C.B. Burckhardt. Speckle in ultrasound B-mode scans. *IEEE Trans. Sonics Ultrason.* 25:1–6, 1978.

[2] D.L. Donoho and I.M. Johnstone. Ideal spatial adaptation via wavelet shrinkage. *Biometrica.* 81:425–455, 1994.

[3] D.L. Donoho. De-noising by soft thresholding. *IEEE Trans. Inf. Theory.* 41(3):613–627, 1995.

[4] V. Frost, J. Stiles, K. Shanmugan and J. Holzman. A model for radar images and its application to adaptive digital filtering and multiplicative noise. *IEEE Trans. Pattern Anal. Mach. Intell.* 4:157–166, 1982.

[5] D.T. Kuan, A.A. Sawchuk, T.C. Strand and P. Chavel. Adaptive noise smoothing filter with signal-dependent noise. *IEEE Trans. Pattern Anal. Mach. Intell.* 7:165–177, 1985.

[6] T. Le, R. Chatrand and T.J. Asaki. A variational approach to reconstructing images corrupted by Poisson noise. *J. Math. Imaging Vis.* (27):257–263, 2007.

[7] J.S. Lee. Digital image enhancement and noise filtering using local statistics. *IEEE Trans. Pattern Anal. Mach. Intell.* 2:165–168, 1980.

[8] L.T, Rudin, S. Osher and E. Fatemi. Nonlinear total variation based noise removal algorithms. *Physica D.* 60:259–268, 1992.

Chapter 4

Mathematical modeling to improve the performance of chemical separation operations equipment

4.1 Introduction

Separation operations are among the most significant operations in the chemical process industries, which are highly significant for the Thai economy, since they include petroleum and petrochemical production, food industries, paints and pigment production, and other chemical production industries. The two most significant separation operations in the chemical industry (in terms of numbers of products which require the operations in their processing) are distillation and crystallization. These processes also account for a significant proportion of the cost of processing the chemicals, and therefore a significant proportion of the cost of the products. Thus, the ability to optimize the separation operations has great significance to the chemical process industry, and such optimization depends on simple but accurate mathematical models of the processes involved. In many cases (for instance for distillation columns operating at steady-state) satisfactory modeling of the systems has been long completed, however there is great need in work in optimization of the processes based on known mathematical models. In other processes (for instance competitive crystallization of polymorphs in a batch crystallizer) optimization is not yet possible because mathematical models for the process are not yet sufficiently accurate. The current project aims to model and optimize the open-steam distillation process, where a mathematical model of the process exists however it has not yet been optimized to obtain a general solution for the optimum reflux ratio used. Another aim is to improve the mathematical modeling of batch crystallization in combination with the polymorph transformation process. An improved mathematical model could be used for process optimization.

4.1.1 Scope and assumptions of the open steam distillation model

The model for the open steam distillation column is based on the constant molar overflow theory assumed in the McCabe-Thiele method of design. This assumption means that the molar flowrates (i.e. flowrate in units of mole/s) of both the liquid and vapor phases in the top and bottom sections of the column are constant values. In this study the steam injected into the bottom of the column is assumed to be saturated at the pressure of the column. Pressure drops inside the column are ignored. The constant molar overflow

assumption is correct when the two species involved have essentially the same molar enthalpy of vaporization under the conditions of the distillation (which is almost always approximately true), the heat of solution in the liquid phase is small (again, this is common), and where there are no heat losses in the column. This reduces the MESH (Material, Equilibrium, Summation, Heat) set of equations to only the material and equilibrium equations, which are more manageable to solve analytically given certain conditions such as a constant relative volatility.

This study assumes that the vapor-liquid equilibrium can be modeled via a constant value of the relative volatility. This assumption is accurate in many distillation systems, however there are obvious exceptions to this, including the ethanol-water system. Thus the results can be used to simulate many industrial systems, but some care is required in their use.

Material balances over the entire column give:

$$F + \bar{V}_{N+1} = D + B \tag{4.1}$$

$$Fx_F = Dx_D + Bx_B \tag{4.2}$$

The top section of the column can be modeled with a solute balance over a finite set of stages (from the top of the column to an arbitrary stage *n* in the top section, above the feed point).

$$y_{n+1} = \frac{L}{V} x_n + \frac{D}{V} x_D \tag{4.3}$$

Which reduces to

$$y_{n+1} = \frac{R}{R+1} x_n + \frac{x_D}{R+1} \tag{4.4}$$

Based on the definition of the reflux ratio, $R = L/D$ and the overall balance which shows that $V = L + D$.

The bottom section of the column is modeled with similar solute balances

$$y_{m+1} = \frac{\bar{L}}{\bar{V}} x_m - \frac{\bar{L}}{\bar{V}} x_B \tag{4.5}$$

The feed mixture must also be added at the most appropriate point of the

column, which is determined via balances around the feed based on the following equation

$$y = \frac{q}{q-1}x - \frac{z_F}{q-1} \tag{4.6}$$

Where q is defined via the following equation involving the enthalpies of the saturated feed, saturated vapor and saturated liquid at the same temperature and pressure (or the fraction of the feed which is a liquid if the feed is a two-phase mixture).

$$\frac{\bar{L} - L}{F} = \frac{H_V - H_F}{H_V - H_L} = q \tag{4.7}$$

The q-line represents the locus of possible intersection points for the top section operating line and the bottom section operating line. This allows for the bottom section operating line to be fully specified given the top section operating line (which only requires the top product composition x_D and the reflux ratio R) and the q-line (which requires the feed composition z_F and enthalpy H_F).

In order to determine the driving force for the mass transfer at any stage in a column (or at any height in a packed column) the equilibrium concentrations must also be known, which is usually given as a function $y^* = f(x)$, where y^* is the equilibrium vapor phase mole fraction for a liquid phase mole fraction of x in the contacting liquid phase. The function depends on the thermodynamics in the given binary system, however a simple and commonly used assumption is that of constant relative volatility, α, where relative volatility is defined (in a binary system) as

$$\alpha = \frac{y^*/(1-y^*)}{x/(1-x)} \tag{4.8}$$

This equation is suitable for use on all stages (n, m).

The equations above can be used for the top and bottom sections of the column, respectively, to obtain the driving force, and using this for the two stages allows for calculation of the total height of a packed column, which we will assume is proportional to the number of stages.

$$L_T = \int_{y_1}^{y_2} \frac{d(Vy)}{K_y a S (y^* - y)} \tag{4.9}$$

The term $V/(K_y aS)$ is a constant known as the height of a transfer unit; what remains (the integral) is known as the number of transfer units. The minimum number of stages is then assumed to be at the reflux ratio giving a minimum for equation (4.9). However there is considerable difficult in solving this system to find a minima.

4.1.2 Mathematical model for the solution mediated transformation of polymorphs

Modeling of particular systems in engineering is done through the well-known population balance equation (PBE)

$$\frac{\partial n}{\partial t} + \nabla \cdot (\mathrm{vn}) + \frac{\partial (Gn)}{\partial L} - B + D = 0 \tag{4.10}$$

n represents the crystal population density, G the crystal growth rate, v is the velocity, L is the crystal size, t is the crystallization time, and B and D are birth and death functions. If the system is well mixed (i.e the properties of the system are the same at any point in the system) than it is possible to use a "well-mixed" form of this balance.

$$\frac{\partial n}{dt} + n\frac{\partial (\log V)}{\partial t} + \frac{\partial (Gn)}{\partial L} = \sum \frac{Q_{in,i} n_{in,i}}{V} - \sum \frac{Q_{out,i} n_{out,i}}{V} + B - D \tag{4.11}$$

In this equation V represents the volume of the mixed suspension, and Q represents and inflow or outflow. This reduces the continuous crystallizer models (which are steady-state) to ordinary differential equations: the assumptions for the batch crystallizer maintain the model as a PDE however. For the batch crystallizer there are no inflows or outflows, and in a carefully controlled batch we can assume that birth and death terms are also zero. In addition, when the change in volume of the species on crystallization is small (as is usually the case) a batch crystallizer operates at constant volume, and as such the second term on the left hand side is zero. In addition, the crystal growth rate is independent of crystal size, such that (in the third term of the left hand side) G can be removed from the differential. Thus the model becomes (for the two polymorphs)

$$\frac{\partial n_\alpha}{\partial t} + G_\alpha \frac{\partial n_\alpha}{\partial L} = 0 \quad n_\alpha(L, t = \mathbf{0}) = n_{\alpha,\mathbf{0}} \quad n_\alpha(L = 0, t) = \frac{B_\alpha(t)}{G_\alpha(t)} \tag{4.12}$$

$$\frac{\partial n_\gamma}{\partial t} + G_\gamma \frac{\partial n_\gamma}{\partial L} = 0 \quad n_\alpha(L, t = 0) = n_{\alpha,0} \quad n_\gamma(L = 0, t) = \frac{B_\gamma(t)}{G_\gamma(t)} \tag{4.13}$$

The driving forces for the crystallization processes are

$$S_\alpha(t) = \frac{C_\alpha(t)}{C_\alpha^*} \tag{4.14}$$

$$S_\gamma(t) = \frac{C_\gamma(t)}{C_\gamma^*} \tag{4.15}$$

These are different functions since the solubility (C*) of the two polymorphs are different. However, the actual concentration of the two polymorphs is the same at any time (since the polymorph molecules are identical in the liquid phase). The growth rate $G(t)$ and nucleation rate $B(t)$ can be determined from the following models

$$G_\alpha(t) = k_{G,\alpha}(S_\alpha(t) - 1)^{n\alpha} \tag{4.16}$$

$$G_\gamma(t) = k_{G,\gamma}(S_\gamma(t) - 1)^{n\gamma} \tag{4.17}$$

$$B_\alpha(t) = k_{B,\alpha}(S_\alpha(t))^{nb\alpha} \tag{4.18}$$

$$B_\gamma(t) = k_{B,\alpha}(S_\gamma(t))^{nb\gamma} \tag{4.19}$$

If the driving force for a polymorph is negative then the growth becomes dissolution. This can only occur to the less stable polymorph (in this case the alpha one).

$$D_\alpha(t) = k_{D,\alpha}\left(1 - S_\alpha(t)\right)^{nd\alpha} \tag{4.20}$$

The model also contains an experimentally determined induction time; the time required from the creation of supersaturation until the creation of viable nuclei. The parameters in these kinetic models can be found from fitting sets of accurate experimental data. The kinetic data needed to parameterize the models for DL-methionine have already been collected in a set of previous articles.

4.2.1 Development of the model and results of the open steam column

It is necessary to first develop the models of the top and bottom sections of the column in terms of the operating parameters for the column. These equations become, for the bottom section

$$y_{m+1} = \frac{C_R x_F R + x_D}{C_R x_F (R+1)}\left(x_m - x_B\right) \tag{4.21}$$

Where C_R is the component recovery, R is the reflux ratio, x_B is the bottom product composition, x_F is the feed composition and x_m is the composition at point m. The top section is already in a suitable form in equation (4.4). The composition in the column at the feed point (the intersection of the two operating lines) can be solved as

$$y_{Int} = \frac{R x_F + x_D}{R+1} \tag{4.22}$$

Then the integral

$$N_{OG} = \int_0^{y_{Int}} \frac{dy_{m+1}}{(y^* - y_{m+1})} + \int_{y_{Int}}^{x_D} \frac{dy_{n+1}}{(y^* - y_{n+1})} \tag{4.23}$$

Breaking this into the two integrals (for the bottom and top sections) we can solve as;

$$\mathrm{N_{OG,T}} = \frac{C_{4n} + \frac{C_{2n}}{2}}{\sqrt{C_{2n}^2 - 4C_{1n}C_{3n}}} \ln\left[\frac{\left(2C_{1n}x_D + C_{2n} - \sqrt{C_{2n}^2 - 4C_{1n}C_{3n}}\right)\left(2C_{1n}y_{Int} + C_{2n} + \sqrt{C_{2n}^2 - 4C_{1n}C_{3n}}\right)}{\left(2C_{1n}x_D + C_{2n} + \sqrt{C_{2n}^2 - 4C_{1n}C_{3n}}\right)\left(2C_{1n}y_{Int} + C_{2n} - \sqrt{C_{2n}^2 - 4C_{1n}C_{3n}}\right)}\right] - \frac{1}{2}\ln\left[\frac{C_{1n}x_D^2 + C_{2n}x_D + C_{3n}}{C_{1n}y_{Int}^2 + C_{2n}y_{Int} + C_{3n}}\right] \tag{4.24}$$

$$\mathrm{N_{OG,B}} = -\frac{C_{3m} - \frac{C_{1m}}{2}}{\sqrt{C_{1m}^2 - 4C_{2m}}} \ln\left[\frac{\left(2y_{Int} + C_{1m} - \sqrt{C_{1m}^2 - 4C_{2m}}\right)\left(C_{1m} + \sqrt{C_{1m}^2 - 4C_{2m}}\right)}{\left(2y_{Int} + C_{1m} + \sqrt{C_{1m}^2 - 4C_{2m}}\right)\left(C_{1m} - \sqrt{C_{1m}^2 - 4C_{2m}}\right)}\right] - \frac{1}{2}\ln\left[\frac{y_{Int}^2 + C_{1m}y_{Int} + C_{2m}}{C_{2m}}\right] \tag{4.25}$$

Where $\mathrm{N_{OG}}$ is a short form for the number of transfer units. In order to obtain the optimum we need to differentiate the sum of (4.24 and 4.25) with respect to the reflux ratio, the controllable variable in the column, and set this differential to zero. This must be a minima in the current problem, for physical reasons. It is not possible to find an analytical solution to this problem unfortunately, however we can numerically solve for particular cases, and an example solution is given in Figure 1. Graphs for further conditions are shown in the main report.

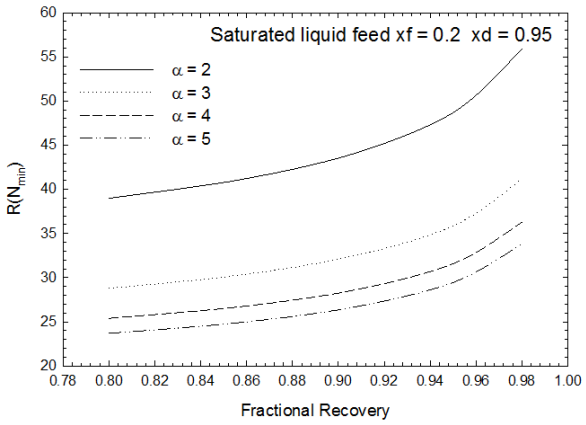

Figure 1. Reflux ratio for minimum number of stages in an open steam distillation column with a saturated liquid feed with solute mole fraction of 0.4. The top product composition is 0.95, and % recovery and relatively volatility as given in the figure.

4.3 Results of the modeling of the solution mediated phase transformation

Two sets of simulations were performed to test the model based on its ability to reproduce experimental data. The results for these simulations are shown in Figure 2 for a batch crystallization where the initial concentration of solute is outside the secondary nucleation threshold of the stable polymorph (causing an instantaneous nucleation of the stable polymorph), and Figure 3 where the initial concentration of solute is within the secondary nucleation threshold of the stable polymorph (causing a delayed nucleation of the stable polymorph). It can be seen that this is well able to reproduce the features seen in the experiment and reproduces the experimental data quite well. Hence the ability to model the physical mechanisms involved is successful.

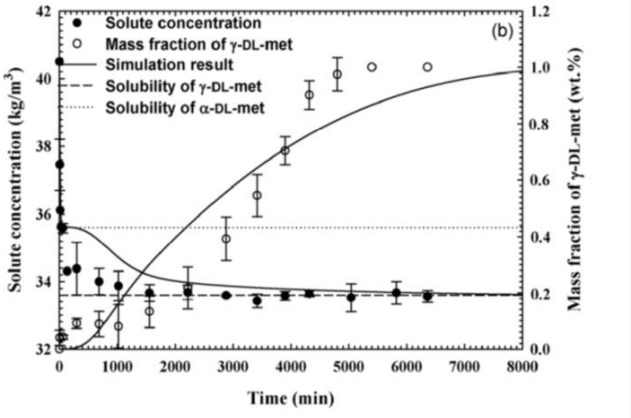

Figure 2. Solute concentration and fraction of γ-DL-met in the crystal phase during the polymorphic transformation for C_0 = 40.5 kg m^{-3} using the model produced in the current work.

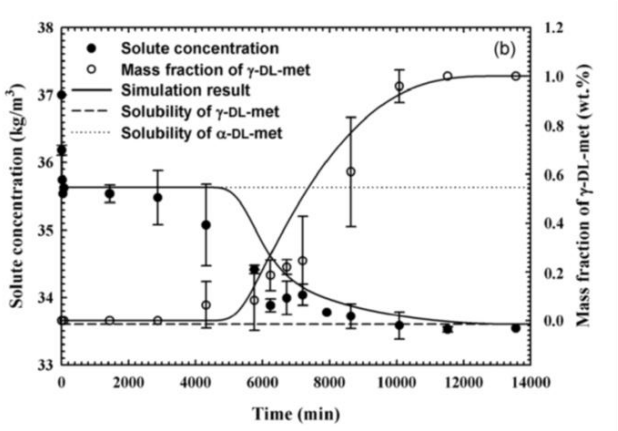

Figure 4. Solute concentration and fraction of γ-DL-met in the crystal phase during the polymorphic transformation for C_0 = 37.0 kg m^{-3} using the model produced in the current work.

4.4 Conclusions

It has been shown to be possible to find the function relating all variables to the number of transfer units (a more convenient task than evaluating the number of stages) and also to take the derivative of this equation with respect to the reflux ratio (and therefore to set this derivative equal to zero to define the reflux ratio at which the number of stages should be a minimum). It has not been possible to solve this equation analytically to give an exact answer for any conditions, however, it has been possible to solve the equation numerically for any given set of conditions.

In the case of the population balance modeling of the solution-mediated phase transformation the model was very successful in reproducing experimental data for the phase transformation. This is a very promising method of modeling and predicting the rates of solution-mediated transformations.

4.5 Acknowledgements

The research was supported by Suranaree University of Technology and by the Office of the Higher Education Commission under the NRU project.

4.5 Outcomes from the research

The research has been published in the following articles;

W. Wantha, A. E. Flood; Population Balance Modeling of the Solution-Mediated Transformation of DL-Methionine Polymorphs, *Chem. Eng. Tech*., 36, 1313–1319, 2014.

A. E. Flood, W. Wantha; Population balance modeling of the solution mediated transformation of polymorphs: Limitations and future trends, *J. Cryst. Growth*, 373, 7–12, 2014.

The work was also presented as a Plenary Presentation in the Asian Crystallization Technology Society symposium in 2012.