

**Research interests** can be summarised as a *Formulation of thermodynamically consistent models for various non-equilibrium processes.*

In detail they are

- *Contributions to frameworks of non-equilibrium thermodynamics*

Focus of V.K.'s research is in formulating thermodynamically consistent models. To this end he develops the general theory of non-equilibrium thermodynamics:

- mixtures [10, 14, 47]
- multiscale thermodynamics [17, 21] including a discussion of role and relevance of entropy and entropy production at different scales [32]
- functional restrictions of phenomenological coefficients and their relation to Onsager-Casimir relations [26, 28]
- a systematic study of irreversibility and dissipation in evolution equations [13]
- generalisation of the widely used exergy analysis pointing out its limits [19]
- a method for the identification of dissipation compliant with purely reversible dynamics [31]
- discussion of a link between stability and dissipation together with symplectic numerical integrators [36]
- a continuum Hamiltonian mechanics formulation containing Poisson brackets with deformation gradients including a link between invariants and conservation laws [42]
- an alternative view on critical phenomena across scales [37]
- a technique providing plausible evolution equations on a lower level of description (dynamic MaxEnt reduction) [33]
- generalization of the dynamical lack-of-fit reduction [41]
- and a general viewpoint on changing levels of description [38]

An overview of our viewpoint of multiscale thermodynamics is in a monograph [30].

As a natural sequel to development of the general theory is applications to various phenomena: transport across membranes, chemical kinetics, the concept of self-organisation (including reaction-diffusion models) being tightly linked to non-equilibrium thermodynamics, a.k.a. dissipative structures, bone remodelling, cartilage.

- *Self-organisation in nature:* Systematic description of self-organisation in nature was initiated by Turing (from mathematical perspective) and then later by Prigogine (from non-equilibrium thermodynamics perspective). Nowadays, it is a widely recognised phenomena ranging across many disciplines. VK's long-term aim is to assess and understand the behaviour and robustness Turing's approach and to amend it if necessary by physically plausible extensions:

- the role of non-diffusibles in Turing's model, large wave number behaviour and the issue of reductionism [6]
- history dependence due to growing domains and a breakdown of the continuum description [24], a general result concerning dilatationally growing domains [46]
- effective diffusion (including interactions with a substrate) rather than actual physical diffusion play a role [18]
- the effect of heterogeneity - the surprising formation of travelling waves [29], piece-wise constant kinetics [35], WKBJ study implying local nature of patterning conditions [40]
- the role of advection in a RD system [27]
- pattern formation in a layered system mimicking experimental set-ups [39]

- isolating a rather robust pattern away from boundary by the choice of boundary conditions [45]
  - revisiting RD model from non-equilibrium thermodynamics perspective yielding Burger’s type equation [43]
  - exploration of intrinsic non-normality of Turing models [23]
  - a recent review of Turing model analysis [44] within a theme PTRSA issue
  - application to understanding hair follicle patterning [22], to Belousov-Zhabotinsky reaction [11]
- *Biomechanics - bone and cartilage:*  
V.K.’s interest in biomechanics dates back to his PhD and Master’s thesis (under the supervision of prof F. Maršík) although the main aims have shifted as indicated in the first point above. The primary interest has been in bone adaptation [2, 4, 4, 5, 8, 12, 15]. Since 2014 V.K. has been working with EA Gaffney (MI platform grant and recently a MCSA-IF project) on cartilage modelling project with emphasis on pathology and experiments (closely discussed with CP Brown). This includes an overview of multiphasic and mixture models in cartilage applications [20], followed by a study pointing out the importance of the appropriate inclusion of heterogeneity of the problem into the model together with the initial and boundary conditions even in standard mechanical tests [34].
  - *PEM fuel cells, membranes:* In cooperation with a very skilled experimentalist JB Benziger (Princeton) we try to isolate particular phenomena in PEM fuel cells such as transport across thin membranes and to understand them from both theoretical and experimental perspective [16, 25, 26].
  - *Chemical kinetics:* The need of understanding mechano-chemical coupling for plausible modelling of bone adaptation led to a development of a rather general theory on this topic [1, 3, 7, 11].
  - *Other:* research project include a result based on MM study group describing placenta development [9].

Some recent works with a sort of public outreach (thanks to Andrew Krause): <https://www.maths.ox.ac.uk/node/30953>, <https://www.maths.ox.ac.uk/node/28581> or see the editorial for a recent [theme issue](#).

Finally, several manuscript are currently near publication:

- a rigorous proof of Liouville-Green (WKBJ) approximation for systems with application to RD problem
- using the Maximum Entropy method to estimate the least biased boundary conditions in mixtures
- SHTC and GENERIC formulation of a binary mixture
- Generalisation of Maxwell-Stefan diffusion to include momentum balances via reduction from a more detailed description

or near submission (available upon request):

- Upscaling of Poisson-Nernst-Planck equation to a macroscale including material heterogeneity and a charge on the solid phase where both knowledge of mathematics and nonequilibrium thermodynamics is necessary for correct upscaled equations (to replace Donnan theory valid only for membranes)
- Asymptotic analysis of qualitative behaviour of a three-sphere linked swimmer near a free surface
- Exact solutions and Lie symmetries of reaction-diffusion system on growing domain
- Stationary shapes of vesicles with surface tension gradients
- A comparison of diffusive (smooth) and sharp interfaces – what is a boundary

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