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RESEARCH

Simulation of Tribosystems and Tribometrology

Modelling and simulation are more and more upcoming tools in various fields in engineering. Most tasks request specialization in terms of the technical background as well as of the mathematical methods used. In this paper an overview is given about some commonly available software tools for simulation with respect to the specific conditions in the field of tribology as an interdisciplinary subject. Aspects of geometry, material characteristics and chemical processes have to be considered. The combination resp. integration of different simulation aims is currently a very interesting task. The focus on processes in the nano domain led to new highly specific simulation tools like molecular dynamics, which enables the simulation of complex tribological processes. Some examples of modelling and simulation are given based on research projects as the are currently running or have been recently finished at the Austrian Center of Competence for Tribology: Targets of these works are problems concerning stresses in tribocontacts, behaviour of lubricants and thermal situations of sliding elements.

Keywords: simulation, oil detachment, TEHD, multi-scale-modelling, tribometrology

1. INTRODUCTION

The development of computer hardware as well as of software tools enables widely spread application of modelling and simulation for many engineering tasks (and of course for other fields of application like medicine, economics, traffic and logistics). Many of the tasks came up due to a sound understanding of the problem behind and the principal knowledge about the possible solution. Yet to a quite considerable extent it is also necessary to contribute experience and skills in the application of mathematical methods and the handling of the concerned tools (i.e. computer software).

Tribology is an interdisciplinary, generic technology with applications in all industrial sectors and our life. Like in medical sciences, tribology is related to more or less complicated systems where it is necessary to be aware of the interrelations within the system concerned and to provide an overview on the whole system. Thus tribology in general and especially tribosystems generate a lot of questions along with the design and improvement of products, modification of materials and coatings, formulation of tailor made lubricants and the necessary technologies behind. These tasks are more and more tried to be solved by application of different simulation processes. This is fairly reasonable considering the costs and risks that may arise during the use of tribosystems.

2. TRIBOLOGY BACKGROUND OF SIMULATION

Understanding of tribological processes enables proper design and selection of materials and as well leads to adequate measures in running the systems.

The major goal of modern modelling and simulation is to provide engineers working in the field of tribology ("engineering tribology") with characterisation of systems' behaviour, valuation of influences and tendencies, detection of critical conditions, and focusing on promising solutions. These measures should be done and to some extent can already be done without the implementation of expensive production lines (which is relevant for mass-produced goods like vehicles – especially

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cars – , household applian-ces, crafts and – with changing relevance – also audio, video, computer, IT peripherals) or without realisation of special, sometimes unique and/or expensive units fabricated in single-part production (e.g. components of aircrafts spacecrafts, power plants, production plants).

The major goal is to predict tribological processes under specific conditions. This can only be done based on a sound tribosystem analyses [1], comprising basic and counteracting bodies (each consisting of bulk material and acting with a special rubbing surface, which is either created during the tribological processes or provided by technological processes), intermediate substance(s) (usually the lubricant), the environment and, of course, stress situation related to functional and structural aspects of a tribosystem. This needs in many cases to consider a multi-scale scope (Figure 1).

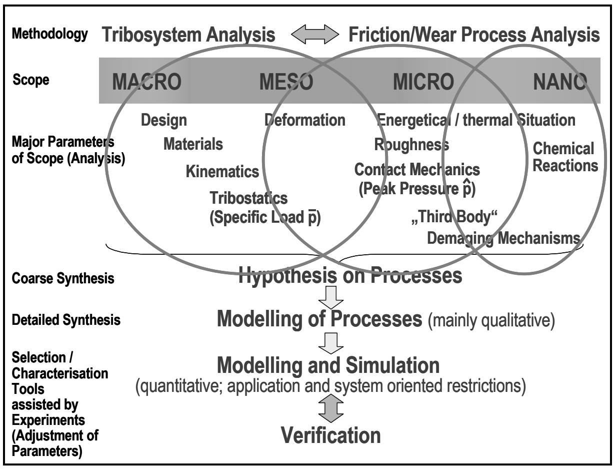


Figure 1. *Modelling and simulation in tribosystems; major parameters of analysis*

In fact, it is necessary to improve our understanding as to tribosystems and the friction and wear in it by using theoretical investigations, yet there will be still the need for accompanying experimental investigations in tribometrology and analytical tool like modern investigation procedures for lubrication engineering, surface characterization and wear analysis.

The knowledge gained in this way in combination with practical experience in the field of Tribology will be applied to improve tribosystems in the industry where the primary tasks are defined:

- Optimising the products and their market position.
- Continuity in the production process and a high level of product reliability.
- Obtaining advanced know-how about effects of friction, wear and lubricants for specific applications, for optimising the design of tribosystems, the improvement of the wear resistance of surface layers, and about the load-carrying capability of lubricants.
- Prediction of service life with respect to fatigue in tribosystems.

Being aware of the main parameters of a tribosystem detailed studies and analyses have to be carried out, based on development and optimisation of simulation models for investigating the influences of the design, surface characteristics and lubrication system.

Besides the capability of advanced measurement and analysis techniques in tribological investigations (especially tribotesting) it is necessary to focus on the processes and effects related to friction and wear on different stages (nano – micro – macro scale). Yet as to systems' design there are – up till now – almost no practical instruments for engineers in order to optimise the design process of tribosystems and thus finally of the concerned tribosystem itself.

Information technology – like in numerous other disciplines – may also assist both, tribological research and tribotechnical practice, in order to increase the efficiency of research work and engineering tasks. Even if the number of parameters controlling a tribosystem is considerably high, more and more solutions will be available for modelling such systems. Further research activities have to focus on suitable modelling tools starting from more or less simple calculations in contact mechanics up to dynamic models for crack propagation, thermal stresses, seizure, and finally (tribo-)chemical reactions.

The general progress of such research work will lead to new tools for the design of tribosystems to improve the reliability of products and guarantee the companies involved a position on the specific market, not at last due to decisive reduction of the R&D period. Data bases and expert systems shall more and more support the finding of relevant material parameters or design solutions for tribological tasks, if suitable structures in terms of the tribosystems and practical tools – especially providing data sharing among institutions of a consortium – are developed and offered.

3. SIMULATION TOOLS – FEATURES OF INTEREST FOR TRIBOLOGICAL APPLICATION

3.1 General requirements

A number of software tools for simulation tasks are offered on the market. These commercially available products are usually designed in order to meet the requirements of a preferably large number of customers or users. Thus on the one hand these programs offer an impressive spectrum of features, yet on the other hand mostly cannot satisfy all the specific needs arising from an application.

General premises for software products in Simulation:

- Enabling of interdisciplinary solutions (which is especially essential in the field of tribology)
- Implementation of capable routines for numerical calculations (e.g. equation solver)
- Flexibility / programmability / scalability
- Easy handling
- Costs and necessary infrastructure (hardware)
- Availability

3.2 Commercial software products and their suitability from a tribology point of view

From the tribology point of view also that products offer capability for simulation tasks, at least for basic problems. Some examples for such versatile tools in terms of tribological tasks are given in the following overview:

ABAQUS (Abaqus, Inc., USA)

Main features

- “Classic” software FEM (finite elemente method) simulations
- Compatibility with industrial standards
- Adaptability in modelling of material characteristics

Applications

- Structural mechanics (mechanical + thermal problems)
- Technological processes (rolling, forming) with strong relation to materials’ behaviour
- Modelling of contacts

MATLAB ® (The MathWorks, Inc., USA)

Main features

- Software tool for numerical calculations
- Complete programming language
- Extensive library providing predefined numerical algorithms

Applications

- Data evaluation and visualisation
- Optimisation tasks, image processing
- Basis for the development of various algorithms
- Programming interface for SIMULINK and COMSOL-Multiphysics

SIMULINK® (The MathWorks, Inc., USA)

Main features

- Software tool for modelling and simulation of dynamic systems with only few degrees of freedom
- Abstract design of models assisted by chart diagrams (graphical user interface)
- Numerical solution of equations of motion (coupled ordinary differential equations)
- Direct integration into MATLAB and COMSOL

Application

- Stick-Slip Simulation

COMSOL Multiphysics® (COMSOL AB, Sweden)

Main features

- Simulation tool – based on FEM (finite element method) – for various physical effects
- grafical pre- und post processor, interactive mesher
- Pre-defined as well as programmable application modi
- direct integration into MATLAB and SIMULINK

Applications

- Structural mechanical effects
- Thermal effects
- Fluid dynamics, fluid-structure interaction
- Electrodynamics
- Combination of several physical phenomena
- Combination of surface and volume related processes

3.3 Advanced simulation tools

FIRE (AVL List GmbH, Graz, Austria)

Main features

- 3D CFD / code for fully unstructured and moving computational meshes (for IC engine development)
- Fully parallized tool (MPI)
- Full multiphase capability (arbitrary number of inter-penetrating phases e.g.: air and oil)

- User-friendly and workflow-oriented graphical user interface; computational meshes are generated with FAME Engine Plus (automatic meshing procedure)
- Fluid-structure coupling and 1D/3D coupling ensures consistent results

Applications
- Complex engine related CFD problems
- Air/Fuel mixture preparation
- Wallfilm behavior
- Flame propagation
- Chemical kinetics in catalysts

EXCITE (AVL List GmbH, Graz, Austria)
Main features
- Tool for concept and design of engines, analysis and optimization of existing power units
- Various contact models and representation of structure components of different complexity and accuracy
- Easy and intuitive handling together with partly automated model creation with powertrain application-oriented pre-/ post-processing reduce overall process time
- Precise and validated physical models enable calculation of realistic dynamic loads and noise levels and allow the design to get close to durability limits
- No limitation on model size thanks to the specific simulation approach
- Interfaces and specific features (fatigue software) enable integration in customer CAE environment

Applications
- Non-linear crank train dynamics
- Thermo-elastohydrodynamic bearing analysis
- EHD piston-liner contact
- Vibration and acoustics of power unit
- Complex tasks comprising structural elasticity and dynamics, energy flow, mixed friction

3.4 Simulation tools for specific tribological tasks

Shifting the scope of tribological investigations to the micro and nano range it is necessary to work on this level in simulation. Lubricant molecules, for example, and their microscopic behaviours at the contacting interface under high pressure essentially influence tribological phenomena. In order to clarify such phenomena, molecular dynamics (MD) code come into play in order to predict tribological dynamics and to study friction resp. traction coefficients. In addition to the atomistic understanding of the tribological dynamics, the electronic-level understanding of the tribochemical reactions is strongly demanded.

However, if simulation of chemical reactions is in the focus, the classical molecular dynamics method cannot be used. Beside this, specific simulations require huge computational resources and costs. Interesting approaches include quantum chemical processes into molecular dynamics simulator tools, and – compared to conventional first-principles molecular dynamics methods – could achieve already considerable acceleration. (e.g. "Tribo-Colors" [2], [3]).

Other simulation tasks concerning tribology on micro/nano level focus on the material behaviour, like crystal plasticity, grain heterogeneities, crack nucleation, partial slip, gross slip etc., which is mainly covered by displacement dynamics (DD, cf. e.g. [4], [5]). Those simulations are for instance useful for technological processes like forming or long time dynamic loading situations (vibrations, fretting etc.). (cf. e.g. [6], [7])
Special software products are available from the market that offer specific capabilities with respect to materials properties (materials laws, mechanical behaviour, creep damage etc.). One example for such versatile tools is **Zebulon** (Northwest Numerics and Modeling, Inc., Seattle, USA) [8] which is a full-featured object oriented nonlinear FEA solver with many special abilities for materials-oriented analysis, yet still being primarily used as a research and teaching tool (available via download from the web). One of the features of Zebulon is its effectiveness for very large nonlinear problems, both in terms of number of degrees of freedom, and number of increments required.

New mathematical concepts have been introduced into simulation related to tribology, like cellular automata (e.g [9], [10]), which possibly enable smart handling of such problems. The necessary computing time is still an important parameter which may restrict the application of simulation tools though capable computer systems or computing methods are available (e.g. [11])

Any way, these types of simulations especially need data input from adequate experimental investigations. In this case it is necessary to perform tests on a series of macroscopic specimens, with various specimen geometries in order to investigate size effect in the contact problem. Careful local observations have to be made to characterise the transformed material microstructure.

Concerning the availability of relevant data (as necessary input for comparison and validation) and the applicability of models it tends to be useful or even necessary to implement multiscale modelling. Finite Element simulations of the tribometrological tests at a macroscopic level enable to describe the behaviour of the tested material as to "calibrate" the specimens, whereas the DD-Finite Element connection provides results dealing with intragranular dislocation distributions.

4. TRIBOLOGY SIMULATION TASKS – SOME EXAMPLES

The following – of course not exhaustive – examples of simulation tasks and applications are taken from currently running or recently finished research work at the Austrian Center of Competence for Tribology.

4.1 Tribological parameters of a paper calender

Task:
The development of a dynamic model of a paper calendar – comprising a hard and a soft roller – is to determine the contact pressures in the roller nip. The slip velocities and the zones of sliding and sticking shall be calculated as well.

Solution/method:
A hard roller and a "soft roller" (roller with roll covering with low Young modulus) are represented by a model, meshing is provided for the soft roller only (Figure 2). Effects (slip parameters) are studied by gradually approaching the hard roller against the soft roller.

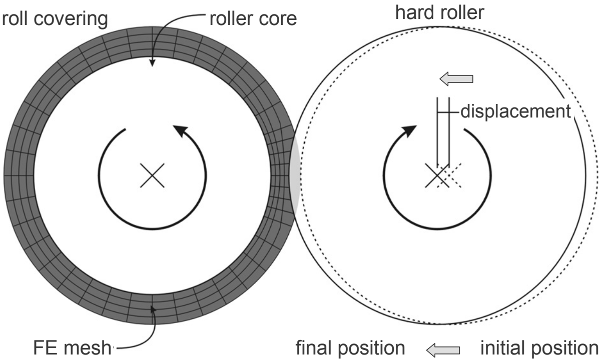


Figure 2. *Paper calendar – modelling of a soft and a hard roller*

Results:
The dynamic modelling delivers stresses (e.g. shearing) in the contact zone as well as slip velocities (Figure 3) of the roller surfaces when passing the nip (Figure 4). The latter identified – depending on the friction coefficient – two zones of sticking.

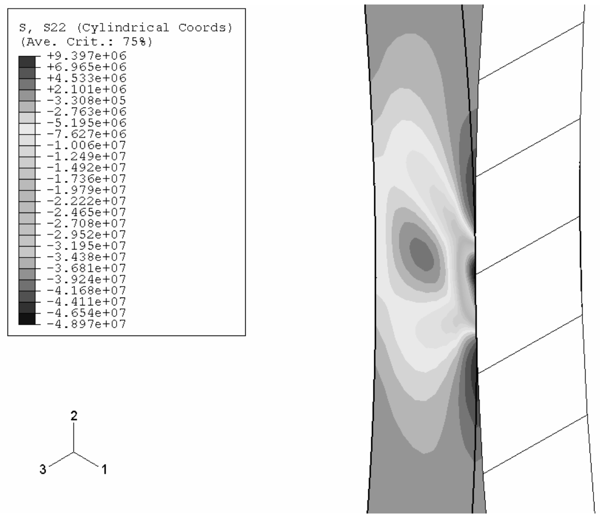


Figure 3. *Paper calendar: tangential stresses in the roll covering*

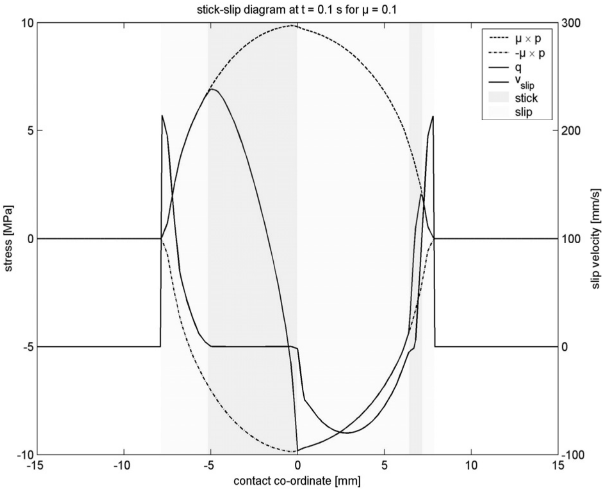


Figure 4. *Calendar nip – different zones of sticking and slipping*

4.2 Numerical simulation of lubricating oil and air flow inside the crankcase of an internal combustion engine

Task:
Due to the movement of crankshaft and piston the formation of oil mist is initiated. This process reduces the availability of the liquid lubricating oil. Blow-by and oil atomisation at piston rings (∏ oil mist) as well as droplet separation from rotating crankshaft web (∏ large droplets, Figure 5) have to be studied.

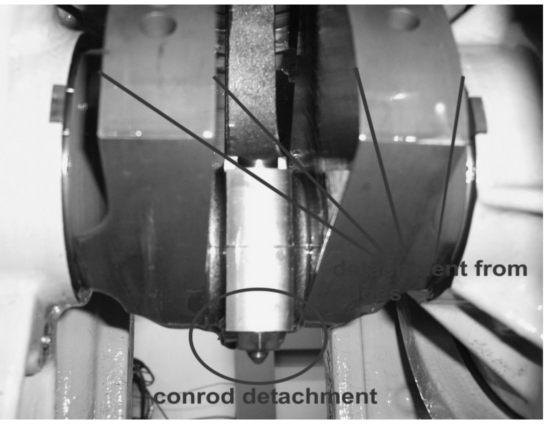


Figure 5. *Crankshaft web – zones with oil detachment*

Solution/method:
Modelling of the flow phenomena is done with the 3-dimensional multi-phase CFD code AVL FIRE (Multi-phase simulation: gas – oil). Slow flow phenomena (condensation, wall film flow) are not considered. Simulation uses a conform moving computational mesh with ~ 160 000 cells, moving piston, rotating crankshaft. The conrod is neglected for this step of modelling. Accompanying tests on a test bench are performed in order to proof correlation between calculated parameters and the system behaviour.

Results:
In Figure 6 are exemplarily presented simulation results of the droplet separation from the crankshaft web. Further studies focused on the development of a droplet size distribution in the crankcase. Boundary conditions for CFD simulation on crankweb edge from rotary atomizer model (disintegration regime, droplet diameter, velocity) (cf. [12]).

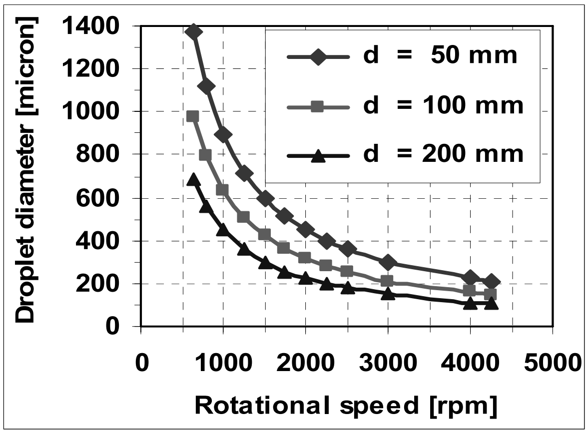


Figure 6. *Calculated droplet diameter depending on different crankshaft web sizes (diameters): Simulation of one revolution at 3000 rpm; Oil: OMV Truck LD SAE 15W-40 at 100 °C*

4.3 Thermo-elasto-hydrodynamic lubrication model for journal bearing including shear rate dependent viscosity

Task:
Advanced simulation of TEHD journal bearing shall include changes in viscosity of the lubricant due to shearing.

Solution/method:
Different viscosity models are introduced into modelling based on AVL EXCITE. The VOGEL equation (considering the influence of temperature), the BARUS equation (considering pressure) and the CROSS equation (introducing the shear rate dependency) are combined to VOGEL / BARUS / CROSS equation:

$$\eta = A \cdot \exp\left(\alpha \cdot p + \frac{B}{C+T}\right) \cdot \left(r + \frac{1-r}{1+\left(K \cdot \dot{\gamma}\right)^{m}}\right) \qquad (1)$$

The behaviour of different VI-improvers is experimentally determined and studied in the simulations.

- PAMA1 – Polyalkyle-Metacrylate-1
- SICP – Styrene-Isoprene-Copolymere

As shown in Figure 7, oils of the same grade with different oil formulations have different shear thinning characteristics.

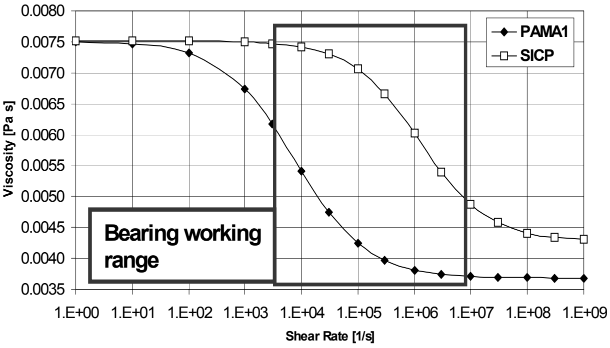
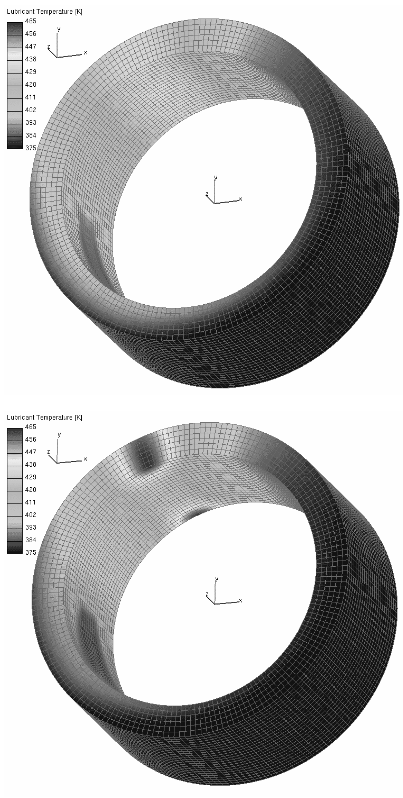


Figure 7. *Shear thinning characteristics of different types of lubricating oils*

Results:
Shear thinning has a strong influence on the lubricant viscosity in the typical bearing working range (shear rate up to $1 \cdot 10^{7}$ s^{-1}). The CROSS equation is applicable for the description of the shear rate influence in the engineering practice. It can be effectively combined with VOGEL / BARUS equation for pressure and temperature dependent viscosity.



Simulation according Vogel/Barus equation

Vogel/Barus/ Cross equation, applied on PAMA VI-improver

Figure 8. *Oil Temperature Distribution*

Viscosity variation due to the shear rate has different influence on various dynamic characteristics: small on peak oil film pressure and strong on minimum oil film thickness, oil flow, peak asperity contact pressure and bearing power loss.

Reduced viscosity of the oil with shear rate dependent viscosity yields lower hydrodynamic load carrying capacity and thus lower minimum oil film thickness. Lower film thickness allows more asperity contact at the edges and this increases the oil temperature at the edges (Figure 8) [13].

Table 1. *Major parameters of simulation with different models and data from VI-improver; POFP peak oil film pressure; PACP peak asperity contact pressure; MOFT minimum oil film thickness*

Calculation results	VB	VBCS SIPC	VBC PAMA
POFP [MPa]	58.7	57.6	58.8
PACP [MPa]	0.34	3.7	8.7
MOFT [µm]	2.5	1.9	1.5
Oil flow [ml/min]	744	792	1272
Max. shear [1/s]	$7.1\cdot10^6$	$8.9\cdot10^6$	$1.1\cdot10^6$
Max. temperature [K]	437	440	465
Min. viscosity [Pas]	0.0036	0.0021	0.0012
Asperity heat [W]	1	13	46
Hydrodynamic heat [W]	347	291	225

4.4 Complex micromodel analysis of wearing contact interfaces

Task:
The behaviour of tribological systems with hybrid lubrication using solid lubricants on graphite basis and/or liquid lubricant can be optimized. This can be achieved by a detailed knowledge of the thermal situation and the transfer mechanisms induced by the tribological stress and consequential material and surface design adaptations.

Solution/method:
The model is based on an assembly of volumes which limit the surfaces taking part in heat exchange and load transfer. Each surface has a set of equations for heat exchange and mechanical loading in the contact. Similarly, transport mechanisms concerning the liquid lubricant, solid lubricant particles and the dissemination of wear particles are considered.

The description of the surface structure is based on statistical methods and the power spectral density function which characterizes the intensity of change of the asperity heights as a function to the roughness frequency.

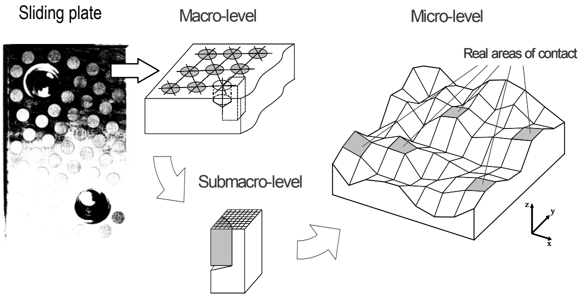
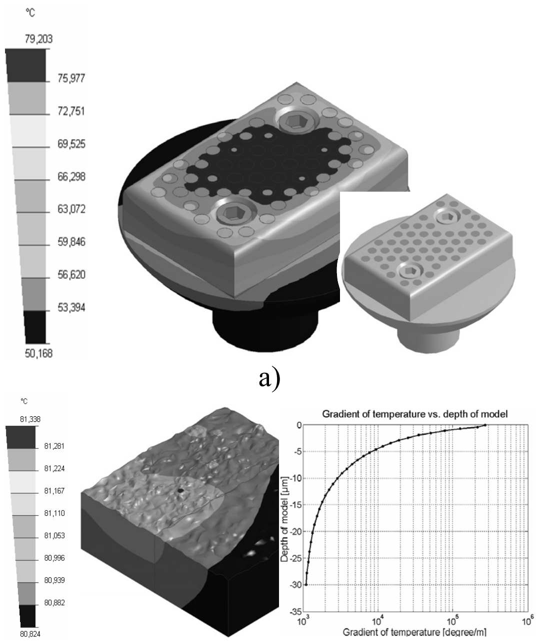


Figure 9. *Graphite-oil-lubricated sliding elements: Multi-level analysis of the contact situation*

Results:
Verification of thermal boundary conditions of micro model can be done by means of thermal macro-simulation (b)

Figure *10*).



a)

b)

Figure 10. *a) Overall thermal situation of a sliding plate (nominal contact pressure 1,6 MPa, sliding velocity 0.5 m/s); b) thermal situation of the surface micro structure*

4.5 Temperature changes of a sliding track (pin-on-disk-tribometer)

Task:
The dynamic thermal situation a sliding track on a disk due to the contact with the pin shall be quantified in order to get information about critical conditions.

Solution/method:
Transient simulation is performed based on FEM-model in COMSOL Multiphysics. In this case –as a special measure – the rotating disk is modelled using a stationary mesh, with the material flowing through the mesh.

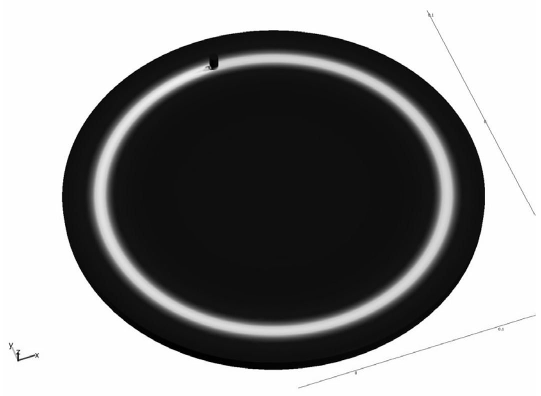


Figure 11. *Temperature changes due to sliding of a pin against a disk (example)*

Results:
Observations / estimations of temperature changes in surface zones due to sliding contacts are possible and enable extended interpretation of tribological experiments (tribotests).

4.6 Investigations on stick-slip effects

Task:
Two AC²T disc-disc-tribometers are suitable to carry out tests on wet friction discs, especially for investigations of stick-slip-phenomena. Similar equipment is used by company partners. Thus it is necessary to compare results from different tribometers. It was aimed at the development of a description tool which enables the valuation of the influence of tribometer design on the results of tribometer tests.

Solution/method:
The basis of the investigation is modelling of the mechanical system (*Figure 12*)

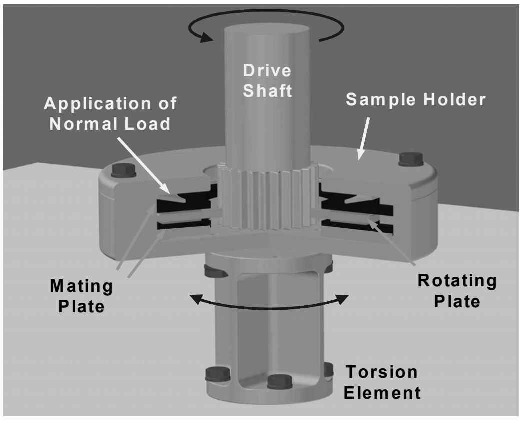


Figure 12. *One-mass-oscillator as used for computational simulation of stick-slip*

The modelled system comprises a sample holder which is connected to the baseplate via a torsion element and where the friction lamellae are axially clamped via disc spring, the disc in the middle position which is rotated via pinion, and the outer lamellae that are fixed in the sample holder

Results:
The influences of the characteristics of the concerned tribosystems on the sensibility to stick-slipping can be at least qualitatively estimated by doing PC assisted parameter studies. In this case synthetic functions for the friction coefficient versus sliding velocity (different slopes) were used. In order to identify the influences the parameters of the tribosystem (I_P … *polar inertia moment*, c_T … *torsional stiffness* and K_D … *damping constant*) were varied.

Though the eigenfrequency according

$$\omega_e = \sqrt{\frac{I_P}{c_T}} \qquad (2)$$

remains equal when both, I_P and c_T, are proportionally changed, the stick-slip behaviour can be changed due to the fact that, for instance, a reduction of the polar inertia moment I_P leads to increased stick-slip sensitivity. Similarly the torsional stiffness influences the stick-slip behaviour, too.

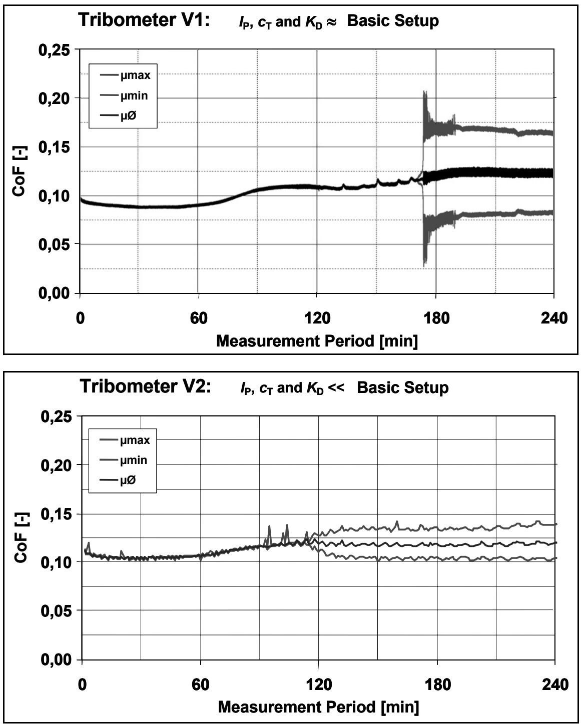


Figure 13. *Comparison of test results from different tribometers*

Tribometer tests (*Figure 13*) showed the influences of the investigated parameters and confirmed the model calculations. [15]

5. OUTLOOK

The performance of computers and the development of software products enabled the implementation of capable simulation tools also for tribological applications. The system behaviour of friction and wear makes it necessary to combine different tools and to consider different scales in modelling. New simulation concepts like molecular dynamics including quantum-chemical effects or mathematical methods like cellular automata may improve the ability of simulation for broad fields of application as requested for various industrial task. The Austrian Center of Competence for Tribology is currently emphasising on the simulation of surface structures and surface effects in terms of tribological processes. A major part of this work is being conducted in the Research Training Network “WEMESURF” (Characterisation of WEear MEchanisms and SURFace functionalities with regard to life time prediction and quality criteria – from micro to the nano range), which could be established within the EU 6th Framework Program [16].

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