xirrus simulation matters – simulation of material properties Factsheet

xirrus simulation offers this product online to you: By the push of a button and by payment in advance you can let calculate material properties of new materials and mixtures.

Requirements

In the following situations the service of xirrus simulation matters is meaningful:

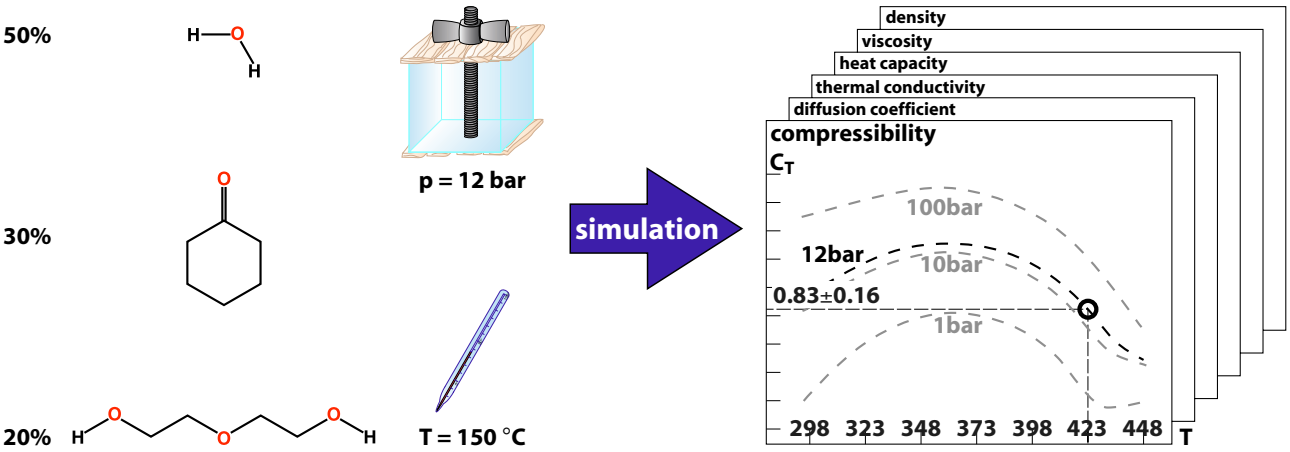
The considered compounds are practically or theoretically known	
type of compound	Organic compounds and polymers (also biocompatible or biological), including silicone as well as most of the existing solvents. • pure compounds, mixtures and additives and functionalizations • often applied chemical elements only (ask in case of doubt) • the mixture contains little or no salts (ions). • The value of pH isn't extreme (between 5-9 in aqueous solution) or irrelevant. • no metallic or ceramic materials
chemical structure	The chemical structure (the connectivity) of the contained components is known, for polymers the approximate degree of polymerisation is known (below 1500 kDa molecular weight). The conformation may be unknown, it evolves and changes during the simulation.
purity	The contained compounds should be close to pure – or the impurities should be known as well and then shall be considered. Impurities in traces can be neglected in most cases. The fractions of individual compounds should be above 1 %. Smaller fractions can often be neglected, or – if expected to be of important contribution to the overall properties – can be included with some extra costs. Please consider any water or solvent fraction as further component. For polymers, the approximate degree of polymerisation (chain length) should be known.
uncertainties	If uncertainties considering the compounds are raised, please contact us directly. With our experienced background we can estimate how to get to the intended goal maybe by applying additional methods.
The requested material property is unknown or unconfirmed	
hypothetical or new material	The material has not been synthetized or mixed, the material is new or has been prepared in a new mixture, characterization hasn't been done yet. The material is expensive or costly in its production. The expected properties shall be derived prospectively in any case.
no measurements	Experiments to derive the missing value are costly or timely or just impossible.
no literature data	No literature data has been found, or not for the desired environmental conditions. Or existing literature data has been doubted.

«Often the knowledge of a "street number" is superior to total ignorance»
Nino Zehnder, Even AG, Zurich, Switzerland

Proceedings and Results

order	Submit us your material data (molecular structures) via online form: **www.xirrus.ch/matters** Please contact us directly for special cases (see footer).	
environment	Adjust the environmental conditions (pressure and temperature).	
property	Order the desired material properties from the following list:	
	density	in [kg/m^3]
	viscosity (shear viscosity)	in [N · s/m^2]
	heat capacity	in [kJ/mol/K]
	thermal conductivity (isotropic)	in [kJ/m/K/s]
	diffusion coefficient	in [cm^2/s]
	compressibility (isotherm) **elasticity modulus**	in [kJ/mol/nm^3] in [kN/mm^2]
	Further properties may be derived as well if circumstances allow. Please ask us directly or use the input field for remarks.	
confirmation and facturation	To eliminate transmission errors, the considered components, environment and ordered properties are confirmed by us after transfer to our simulation software.	
prepayment	You'll have to pay us the necessary fee in advance. The simulation starts, as soon as the payment has been booked on our account.	
simulation	xirrus simulation matters simulates your material at defined environmental conditions (pressure, temperature, provided by you) in microscopic adequate size and time, analyses the results and calculates the required properties.	
period of delivery	Normally, you can expect the result within several days. Since simulation, analysis and statistics on a molecular level demands for much computational power, sometimes it can last for days or weeks until the result is calculated.	
result accuracy	The achievable accuracy of such simulations is limited methodically (e.g. deviations of the density up to 5 %). The significance is, as well as with experiments, reduced by the limitations of the models used.	
guarantee	At proven deviation (of more than a factor of 10 of in similar cases standard deviations) by at least three independently published, but similar literature data [verifiable sources] and your announcement within two months after delivery, you'll get your cash back. Such a case would help us detect invalid model limits and consider the models again in case of comparable requests.	

Example of a property derivation by simulation



Why xirrus simulation matter^{s}*?*

enlightning	Many material properties aren't linearly coupled to their environmental conditions, which makes extrapolation rather difficult, especially if not enough indications do exist.
convenient	High temperatures or pressures demand for high performance equipment for experiments and measurement technology. Not every situation allows for this equipment or measuring devices.
prospective	Exactly in the planning and development phase new materials can be analysed virtually and significantly accelerate your development.
simple	Order online: **www.xirrus.ch/matters**

Online order of xirrus simulation matter[s]

To order xirrus simulation matters online, the following steps and thinking is done:

Definition of substance, and substance mixture

You have three possibilities to identify the substance:

- Enter a distinct name
- Specify the SMILES-string, a characters language for chemical formulae
- Draw the chemical structure in the formula editor

Distinct chemical name

Whenever possible, please use the systematic, chemical nomenclature of IUPAC (as e.g. 2,3,4-Trimethylhexane) or a distinct trivial name (e.g. Norbornane) to allow us for distinct identification of your compound. Names according to INCI, as applied for cosmetic compounds, may also be used.

Please avoid unclear trivial names or abbreviations.

SMILES-string

If you don't know the SMILES-string or the chemical name, but you could sketch the molecular structure, simply draw the corresponding molecule with the editor for the individual component. By closing the editor a SMILES-string will automatically be created.

Polymers: For polymers draw the monomeric unit and give the replication of the unit on both sides by attaching the special atom type R. This works by selecting the end with the selecting rectangle or lasso, such that the ending atom is selected only. The pseudo-atom R is found in the menu atoms, under pseudo-atoms.
The SMILES will contain * [and evtl. a mass, which can be ignored] for the placeholder atom. Don't forget to define the polymerisation degree in the field for the name of the component.

Biopolymers (peptides and genetic fragments) are well suited for this type of simulation, but long sequences would be out of range of this scope of an order. If you have special questions about interactions or properties of biopolymers, please feel free to contact us directly and let analyse your case individually.

Additional components

Just click on the corresponding link for another component of a mixture and a new input section will open. You can enter as many components as you need, but be aware of the augmenting price for the more complex system.

For further components you proceed equally. Additionally you have to provide either the molar ratio compared to other components in integer units, as you would prefer for chemical reactions, or simply declare the percentages of masses, such that the sum will be 100 %.

Be aware, that no component should fall below 1 % of mass fraction, since we should have a certain statistical weight in the simulation to get a significant influence in the calculation of macroscopic properties.

Chirality

We offer the possibility to consider chirality. This may be of importance, if you have added chiral components. In the materials branch this is rarely the case, in the bio- and medical branch (life-science) it may be significant and very important.

If you're not aware of chirality, please choose no.

If you state we should consider chirality (handedness, enatiomorphy) it makes simulation more complex. The consideration of chirality only is meaningful, if it contains chiral components. Our recommendations what are best choices you can read in the online help.

Environmental conditions

Define here the temperature and pressure at which material properties should be derived. Normally, material properties are depending on environmental conditions (e.g. a polymer gets softer when heated).

You can define several different environmental conditions, e.g. to simulate a series of measurement. This will track off several separate simulations of the same substances at the named environmental conditions, i.e. not a simple extrapolation. For new materials with unusual properties this is very important (e.g. if they get harder when heated).

Desired properties

Finally choose, which properties you'd like to derive. In the online help, the units are named, in which we derive the results.

Check input

Click here to check your entries for missing data. Missing or inconsistent entries will be highlighted. The check will also run automatically when submitting your order.

Remarks

Enter additional remarks considering your order or your materials, or add your questions we should discuss.

Addressing

Please enter who shall get the confirmation and the results.

Basics of xirrus simulation matter^{s}

simulation	xirrus simulation matters simulates your material at defined environmental conditions (pressure, temperature) in microscopic adequate size and time, analyses the results and calculates the required properties. The simulation runs under thermodynamic equilibrium, at constant pressure and constant temperature (i.e. NPT-ensemble). The predefined values correspond to the standard conditions of a laboratory.
molekular dynamics simulation	xirrus simulation matters is based on classical molecular dynamics simulation. All molecules including their atoms, bonds and physical models with mobility of conformations and physical dynamics are calculated as the thermal velocity would demand during time. Simply spoken, the atoms play billard in 3D. The offered properties of materials can be calculated from the molecular motions by statistical thermodynamics. Yes, it is quite complex to understand. Therefore we do not want to explain you the use of the programs, but help you to take the advantage out of it. For productive software we use GROMOS and Gromacs. These are well established products in the scientific community.
force-field (model)	The molecular models are built on atomic particles and molecular fragments. They have been developed over years and fine-tuned. We apply GROMOS-force-fields and extensions.
phase, state of aggregation	The state of aggregation (solid, liquid, gaseous) of a compound depends on the environmental conditions (pressure, temperature). It establishes itself within the simulation. We start with a homogeneous, randomly generated mixture – as it may occur in reality too.
expertise	Much knowledge and experience of xirrus goes into the derivation of new models and new combinations of models, as well as into the parameters and our services.
special cases	We're happy to establish simulations for you, that would deviate from the standards (e.g. non-equilibrium-simulations, or constant volume instead of constant pressure). Please feel free to contact us to discuss the details.
other requests	We help you to solve molecular based, or particle based complex problems by understanding the systems. We'd like to discuss possibilities personally with you and to introduce our methods. A close insight about our work you get from our video on www.xirrus.ch/video.

