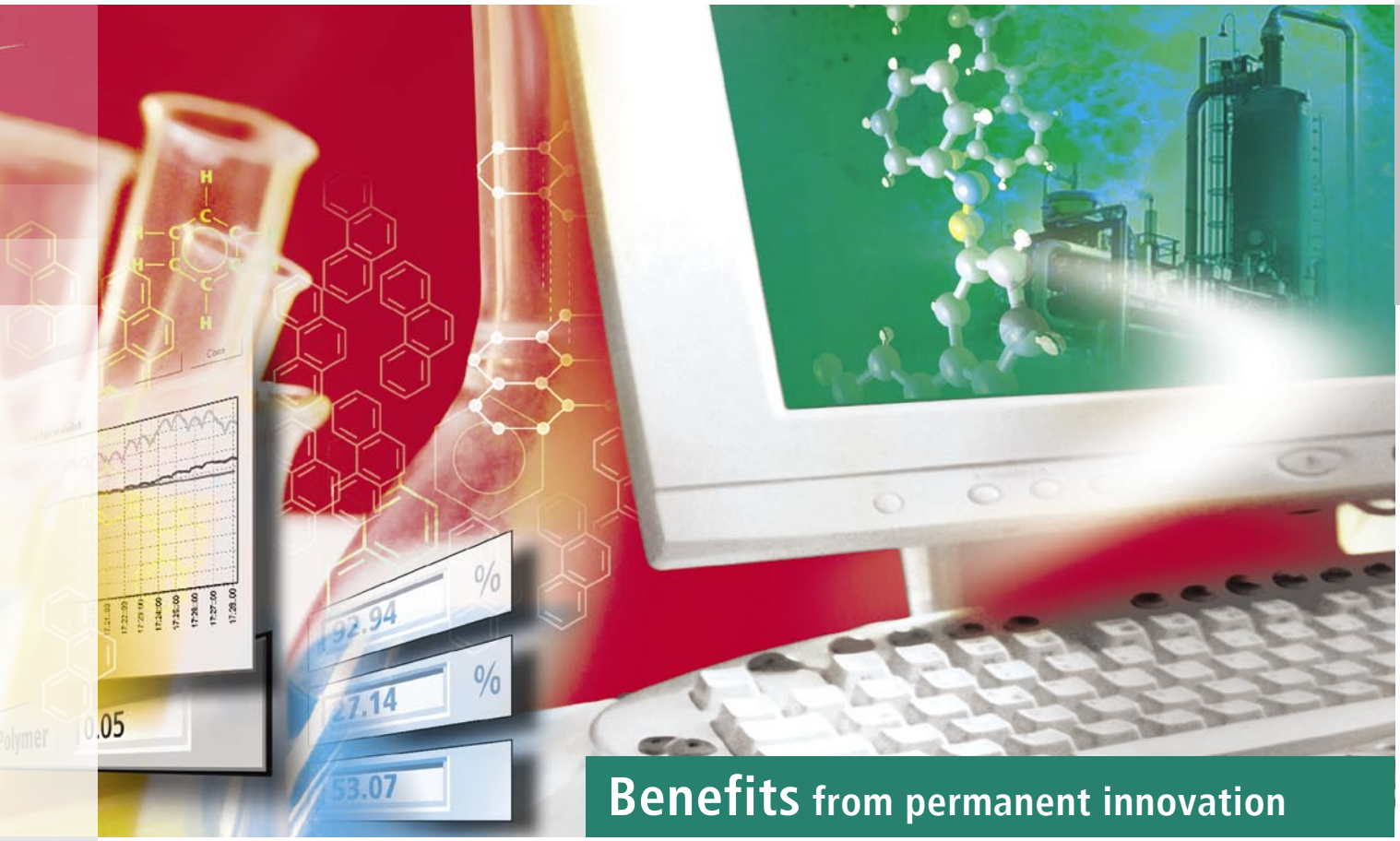
CiT Dr. M. Wulkow
Computing in Technology



Benefits from permanent innovation

CiT

CiT SOFTWARE

High-end solutions for extraordinary challenges

Simulation in Chemical Engineering

CiT – Software, Service and Mathematics for Innovative Modeling

CiT provides advanced modeling software and technologies for the chemical, biotechnical and pharmaceutical industry.

CiT's successful philosophy is to combine leading mathematical algorithms and modeling concepts with highest software standards – performance and ergonomics – and best possible versatility, support and service.

Users of CiT software need not be mathematicians or programmers and they don't have to derive equations or algorithms. We want you to do what you know best – think about your process!

Because of their special modular approach and the incorporated script language, all CiT tools allow the extension of current knowledge – there is no need to stop at current barriers!

Some key facts:

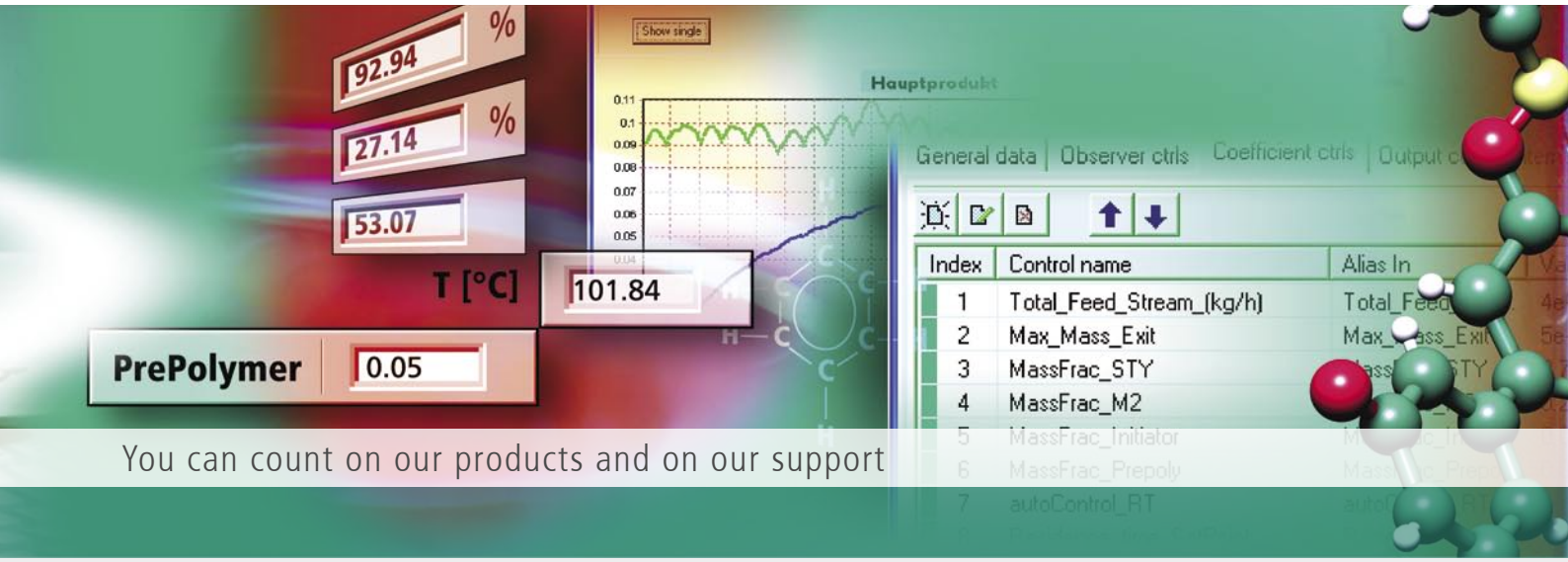
- CiT has more than 100 industrial clients around the world
- Hundreds of innovative publications and projects are based on CiT software
- With PREDICI – considered as quasi-standard for polymerization modeling – and PARSIVAL – the reference solver for particle size distributions - CiT is the leading provider of software for the modeling of population balances
- CiT software has entered education in chemical engineering departments of universities worldwide
- CiT is permanently engaged in research projects – from mathematical concepts to highly-sophisticated modeling – and cooperates with leading research institutes

PREDICI

The leading software package for the modeling of polymerization kinetics and processes

- Rigorous computation of full molecular weight distributions by CiT's unequalled Galerkin h-p-algorithm
- Easy-to-use treatment of virtually all kinds of polymerization processes – think in terms of phenomena and reactions and follow your ideas
- Comfortable recipe handling and powerful parameter estimation – design your MWD
- Continuous, semi-batch, batch and tubular reactors, cascades and loops, phases and thermodynamics – it's not only kinetics
- Outstanding parameter estimation tools, especially the solving parameter correlations can be used for even

• High-temperature polymerization of Methyl Methacrylate • Nitroxide mediated living free radical polymerization of Styrene • Characterization of catalysts • Kinetic simulation of living carbocationic polymerizations • Reversible addition-



You can count on our products and on our support

PRESTO-KINETICS

The easy-to-use tool for advanced kinetic modeling

- Unique modular approach to chemical kinetics
- Selection of high-quality DAE-solvers
- Comprehensive parameter estimation for large data sets
- Bio kinetic modeling
- Catalyst modeling
- Dynamic treatment of tubular reactors using the PDE-version of CiT's h-p-method – rely on high accuracy methods

newest 'reduced directions algorithm' for the most complicated models

PARSIVAL

The reference tool for population balances for all kind of particle processes

- Solver for particle size distributions based on continuous Galerkin h-p-method
- Modular treatment of all phenomena, e.g. nucleation, growth, attrition, agglomeration, breakage, classified streams
- Treatment of continuous and batch reactors as well as of flowsheets
- Parameter estimation even for full particle size distributions
- Applications range from all kinds of crystallization processes to dispersions, precipitation reactions and mill characteristics to aerosol modeling, polymer particles, nanostructures and bio pellets.

OBSERVER

The new tool for model predictive control and process intensification in connection with PREDICI, PRESTO-KINETICS and PARSIVAL simulations

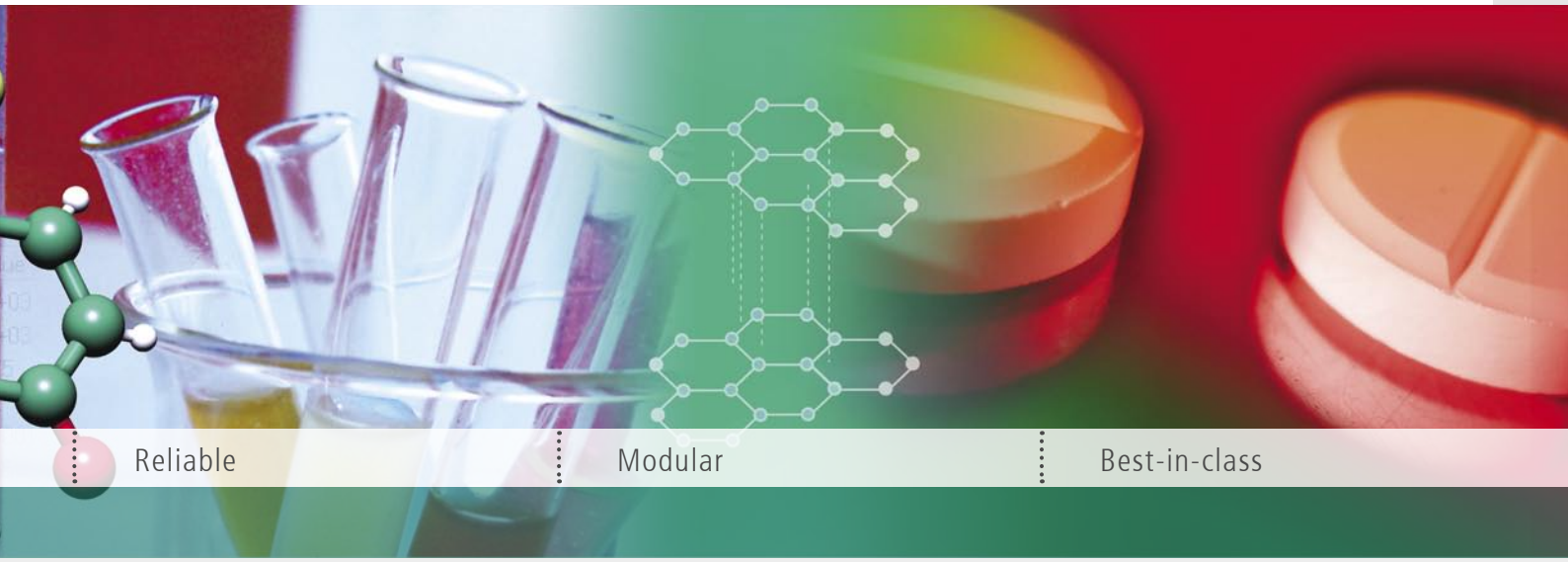
Real-time simulation based on complex models

- Online training
- Process observation based on PCS data
- What-if simulations parallel to live process
- Process optimization
- Open and flexible interface, easy-to-configure, no programming
- No re-engineering of models necessary
- Very robust and stable, has been proven by months of permanent operation in plants

BENEFITS

- Improved process operation
- Training for 'what-if' scenarios
- Deeper insight into processes
- High level acceptance of modeling projects

fragmentation chain-transfer (RAFT) copolymerization of Vinylidene Chloride and Methyl Acrylate • Modeling of Free-radical Crosslinking Copolymerization of Acrylamide and Methylenebis(acrylamide) for Radiation Dosimetry • Atom Transfer radical polymerization • QMOM • Nitrification in bio filters • Virtual lab for pharmacokinetics • Branched architectures in radical polymerization systems • LDPE product properties and molecular structures • Fractal dimension in aerosol process simulations • Regeneration of coked catalysts • Grinding and agglomeration in stirred media mills • Effect of Additives on TEMPO-Mediated Alkoxyamine Isomerizations • and many more



Reliable | Modular | Best-in-class

PRIAMOZ

Optimization and Optimal Control for PREDICI models

Possible objectives

- Conversion, mean values, composition, rheology, general product properties
- Process time (time optimal control)
- Molecular weight distributions

Possible controls

- Temperature profiles
- Recipes
- Feed profiles
- General model parameters

BENEFITS

- Optimization of real process time
- Optimization of product properties
- Optimization of recipes and control

LAMDA-S

LAMDA-S is a new database for experimental data in chemical engineering, containing all of our experience in data handling, modeling and simulation and software engineering.

Features:

- Comfortable search engine, configurable for high efficiency
- Online graphs for quick check of search results
- Export of search results to Excel
- Flexible input based on open forms for any type of data and skill of user
- Extendable to all kinds of physical properties, physical units, measurement attributes and input styles
- Client-server structure with user and administrator versions for safe and controlled handling
- XML-based, safe for future, data are stored for a long time, not dependent on OS or database engine

Additional features:

- Input and search possible for an unlimited number of single databases
- User-right's administration
- Direct communication between lab and client

BENEFITS

- Professional storage of valuable data and their retrieval
- Own standardization of data capture

The earlier you start with a systematic administration of your expensive and valuable data, the earlier you will receive the pay-back.

With LAMDA-S you will not only have the answer in a second, but all matching data at hand for further treatment.

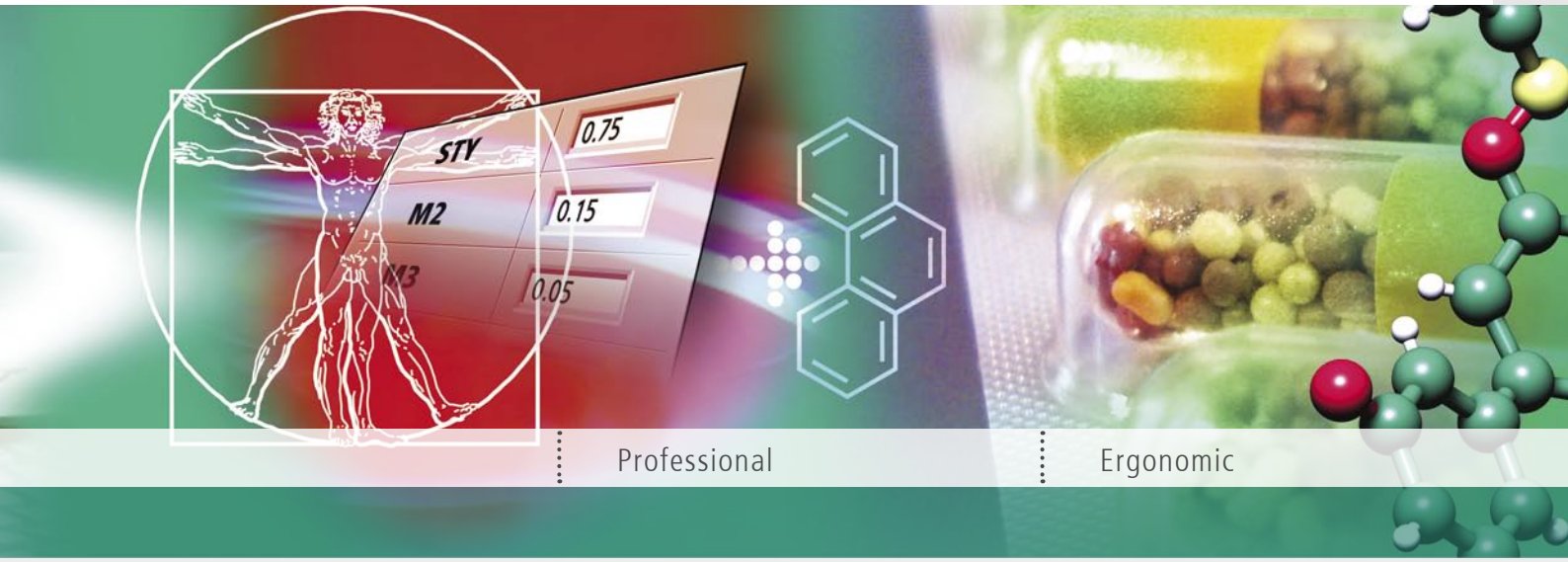
Now available:

LAMDA-S-Express is a free adjunct to **LAMDA-S** which supports data acquisition from external clients.

„Do we have experimental data for substance M at temperature T between 60 and 85 °C, measured with equipment X or Y, ordered by production site B between 2013 and 2016?"

Imagine how many data are lost in labs, because they are not treated as information but as plain, free-style documents.

The result: even if such files are linked to a documentation system, the access to the meaning of the data is lost or difficult to retrieve an to process.
With LAMDA-S you can store data and get them back.



Professional

Ergonomic

A virtual laboratory for innovation in pharmacokinetic modeling

Cit does not only produce standard software, but has successfully performed special software and research projects for the last 20 years

- Water quality management tool for river basins
- Supply chain management tool
- Chemical property administration software
- Training simulators for new technologies – model development and software
- Joint work with clients on models for catalysts, polymers, crystallizers, coupling to CFD simulations
- Special cooperation with the Sonderforschungsbereich 578 "From Gene to Product", TU Braunschweig
- Safety computations for polymer processes

MEDICI-PK

MEDICI-PK is new and innovative and relies on over 15 years of experience in the development of software structures and numerical applications.

The close cooperation with universities ensures (as for all of our products) a sound scientific foundation and permanent development.

Software in terms of the specific needs in physiologically based pharmacokinetic modeling

- Modular, transparent, application specific and user-friendly
- Using the 'modular design principle'
- Employing state-of-the-art scientific numerical algorithms
- Providing comfortable output, online graphs and derived data (AUC), Excel interface
- Direct access to and editing possibility of all parameters and models
- Integration of SBML biology models
- Developed in close cooperation with the Junior Research Group ‚Computational Physiology'

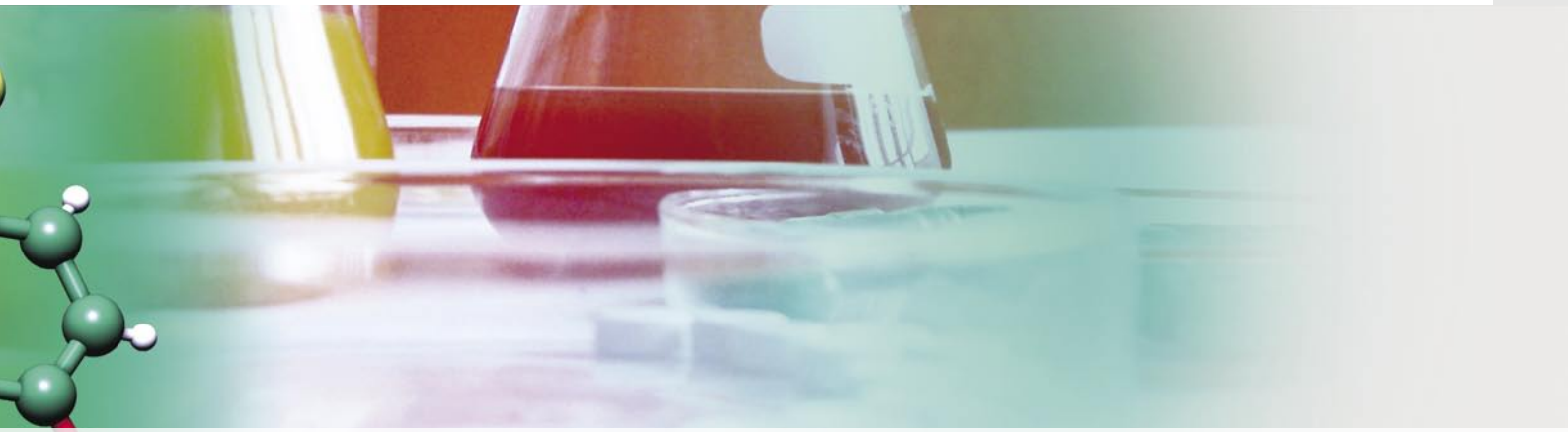
Freie Universität Berlin and MATHEON

BENEFITS

- Increased insight into pharmacokinetic processes
- Support of the powerful combination of in vitro experiments and in silico modeling
- Increasing knowledge and predictivity
- Support of model building and hypothesis testing

Further benefits of CiT's basic simulation tools

- **Correct, reliable and efficient modeling possible by chemical experts and process engineers**
- **Accelerated realization of new ideas**
- **Reduced experimental costs**
- **Shorter payback times and better control of processes and product properties**



Contact and licensing

Flexible license options for CiT software:

- Permanent single and group licenses
- Temporary licenses
- Evaluation licenses
- Special academic license models

Additional services:

- Individual software development
- Special modeling consulting in various fields
- Modeling projects

CiT is the only distributor for all its products.

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