Fluid Work Bench® –

Code for calculation of Thermophysical, Transport and Optical properties of gases, fluids and plasmas
**Calculated properties**

- **Thermodynamic properties:**
  - Equilibrium composition, \( n_i \)
  - Constant pressure heat capacity \( C_p(T,P) \)
  - Enthalpy \( H(T,P) \)
  - Entropy, \( S(T,P) \)

- **Transport properties:**
  - Viscosity coefficient \( \mu(T,P) \)
  - Binary diffusion coefficients \( D_{ij}(T,P) \)
  - Thermal conductivity coefficient \( \lambda(T,P) \)
  - Electrical conductivity \( \sigma(T,P) \)

- **Optical properties:**
  - Absorption coefficient \( k_{abs}(T,P) \)
  - Net Emission Coefficient \( \varepsilon_{net}(T,P) \)
  - Radiative heat conductivity \( \lambda_{rad} \)
  - Refraction index
  - Radiation spectrum

**FWB Highlights**

Fluid Workbench (FWB) is designed to calculate:
- radiation
- transport
- thermophysical properties of gases, fluids and plasmas

**Applicability range:**
- Pressure: up to 1000 bar
- Temperature: up to 100000 K

**Applications:**
- combustion
- high pressure discharge
- high temperature chemical technologies
- metallurgy
Format of Data generation and data transfer to other codes

- **Look-up tables in ASCII format**
  - Transport properties
    - Optical properties
  - Parallelization by multiprocessor structure

- **Direct interface to commercial CFD codes**
  - FWB: calculation of Thermophysical, Transport and Optical properties of gases, fluids and plasmas
  - DB: Elementary properties of atoms and molecules
  - UDF: read data and data transfer
  - CFD codes: Fluent, OpenFoam, Comsol
Fluid Workbench functionality and data flow

Fluid Work Bench functionality

Calculating properties:
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- Heat capacity \( C_p(T,P) \)
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Ray Tracing:
- Spectrum generation
- Integral radiative characteristics

Heat & Mass Transport
- Heat Flow
- Mass Flow

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Optic properties:
- Broadening
- Cross sections
- Rate constant

Processes Data Base
- Thermo properties
- Electr. levels structure
- Interaction potentials

Substances Data Base
- Broadening
- Cross sections
- Rate constant

Post Processing

Ray Tracing:
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Heat & Mass Transport
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Look-up tables

CFD codes
- ANSYS
- Fluent
- OpenFOAM
- Comsol

Fluid Workbench (FWB) functionality and data flow:
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- Cross sections
- Rate constant

Transport properties:
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Look-up tables
Extended set of models and modules for properties calculation and postprocessing

- Absorption coefficient calculation
- Refraction index calculation
- Thermo prop. for non-equilibrium
- Thermo prop. for equilibrium
- Transport properties calculation

- Average absorption coef. calculation
- Fitting of absorption coefficient
- Net Emission calculation
- Rosseland conductivity calculation
- Spectrum calculation
- Many parametric calculations
- Optimization of wavelength mesh
Easy to use interface & parallelization of massive calculations

FWB: calculation of Thermophysical, Transport and Optical properties of gases, fluids and plasmas
Easy to use interface & parallelization of massive calculations

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Easy to use interface & parallelization of massive calculations

- Transfer thermodynamic data
- Calculate composition in LTE
- Transfer initial composition
Easy to use interface & parallelization of massive calculations
Easy to use interface & parallelization of massive calculations

FWB: calculation of Thermophysical, Transport and Optical properties of gases, fluids and plasmas
Easy to use interface & parallelization of massive calculations
Collection of properties of more than 5000 species

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Electronic levels</td>
<td>energy structure</td>
</tr>
<tr>
<td>Thermodynamic data</td>
<td></td>
</tr>
</tbody>
</table>
Data of more than 20000 elementary optic and 120000 kinetic processes

Transition parameters for
• atoms
• molecules

More than 20000 electronic transitions

more than 120000 elementary electronic and heavy particle elementary reactions

Broadening characteristics:
• resonance,
• Van der Vaalse
• Stark,
• Quasistatic
• .....
### Data for other potentials:
- **Modified LJ (m-6):**
- **Buckingham – Corner:**
- **Stockmayer:**
- **HFD-B potential (Aziz):**
Approaches for transport properties calculations

Accurate formulas of Chapman-Enskog method with account for higher approximations are implemented in FWB and used in all calculations under LTE conditions.

**Approximation:**

- Viscosity $\mu$ is calculated in the second approximation ($\xi=2$).

- Translational thermal conductivity $\lambda^{tr}(\xi)$, electrical conductivity $\sigma(\xi)$ are calculated in the second or third nonvanishing approximations, depending on data available for interaction potentials.

- Binary diffusion coefficients $BD_{ik}(\xi=1)$.

- Multicomponent diffusion coefficients $D_{ik}(\xi)$, $\xi=2$ or 3, are calculated just to use them in the formula for $\sigma(\xi)$.

- Total thermal conductivity $\lambda_{eff} = \lambda^{tr} + \lambda^{int} + \lambda_r$

- Effective heat capacity $C_{peff} = C_p + C_{pr}$

**Potentials & Data Bases:**

- Pirani Potential (neutral, neutral-ion)
- Polarization Potential (elastique)
- L-J, Buckingham-Corner, Stockmayer, Aziz Potential (neutral-neutral)
- Screened Coulomb Potential
- Devoto for Charge exchange
- Collision Integrals Tables for e-neutral
- Tabulated Potentials
Example: Thermal conductivity, viscosity and electrical conductivity of Air
Example: Thermal conductivity, viscosity and electrical conductivity of Argon
Approaches for optic properties calculations

**Atoms:** generalized approach of bond-bound transitions

**Atoms:** Photoionization continuum: Kramers-Unsold-Biberman model, tabulated cross section

**Molecules:** Born-Oppenheimer + Frank-Condon approximations for bound-bound transitions

**Molecules:** Quasi-classical approximation of wave functions for vibrational spectrum.

**Molecules:** Hönl-London factor approximation for rotational spectrum

**Broadening:** resonance, Doppler, quasistatic, impact, Stark, Van der Vaalse, ...

**Approximation:**

\[
W(nl\gamma, n'l'\gamma') = \frac{2e^2 a_0^3}{3mc^2} \frac{\hbar a_0}{R_y} (2l + 1) C(l\gamma, l'\gamma') (R_{n\gamma}^{l\gamma})^2
\]

\[
k_{in}(\omega) = \frac{16\sqrt{2\pi} a e^4 Z^2}{3\omega^3 \sqrt{3n kT}} GN^2 N \exp\left(\frac{\hbar a_0}{kT}\right)
\]

\[
A_{\gamma,\gamma'\gamma,\gamma'} \cdot \frac{4}{3g_i} \left(\frac{e^2}{\hbar c}\right)^3 \cdot \omega^3 \cdot \left| \langle v(i) | D_y(R) | v'(j) \rangle \right|^2 \cdot S_{\gamma\gamma'}
\]

\[
R < R_c^{(s)} \quad \Psi'(R) = C^{(s)} \sqrt{\frac{k}{k^{(s)}}} \cdot \left[ Z^{(s)}(R) \right]^{1/4} \cdot \text{Airy}[-Z^{(s)}(R)]
\]

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\]

A convolution of a Gaussian and a Lorentzian, Voigt:

\[
V(x; \sigma, \gamma) = \int_{-\infty}^{\infty} G(x'; \sigma) L(x - x'; \gamma) \, dx'
\]
Examples: optical properties of Air

Mean absorption coefficient of Air, 75 atm

Net emission coefficient of Air, 1 atm
Examples: Absorption coefficient & Refraction index

Absorption coefficient of Cu

- Klock paper, Continuum
- Total, Klock paper
- Calculation

Refraction index of Xe

<table>
<thead>
<tr>
<th>λ, nm</th>
<th>f_ik(Bideau)</th>
<th>f_ik(NIST)</th>
</tr>
</thead>
<tbody>
<tr>
<td>146.9</td>
<td>0.268</td>
<td>0.273</td>
</tr>
<tr>
<td>125.6+129.5</td>
<td>0.295</td>
<td>0.196</td>
</tr>
</tbody>
</table>

n-1, T=273 K, P=1atm, Kintech calc.
n-1, T=273 K, P=760 Torr, Bideau paper

\[ \sum f_{ik} = 1.6 \]

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Other products of Kintech Lab

**Chemical Workbench®**
- Comprehensive library of reactor models for simulation of multi-phase thermodynamic equilibria, homogeneous gas phase, heterogeneous and non-equilibrium chemical active plasma kinetics
- Model explorer for building multi-stage process workflow flow as a chain of reactors with recycles
- Extensive set of tools for manipulation and analysis of kinetic mechanisms: comparison, analysis, reduction
- Multiple options for reaction-rate approximations in kinetic simulations, including user-defined expressions
- Customizable and flexible post-processing tools: units conversion, user-defined results processing, plot templates
- Integration with databases on thermodynamic properties of substances, kinetic data, individual chemical mechanisms

**KintechDB®**
- Thermodynamic property data for 4500 substances
- Physical properties for 1700 species
- Molecular data for 800 species
- Rate coefficients for 6500 gas phase and liquid phase reactions
- Automatic data transfer from Database to Chemical Workbench® calculations
- Saving data from Chemical Workbench® to the Database for future use

**Mechanism Workbench®**
- Fully automated – no background in mechanism reduction methods is required. Fully automatic mechanism reduction procedure based on proprietary algorithms and modern mechanism reduction techniques
- Less work for most popular applications – templates of mechanism reduction for IC engines and GT combustion and emissions applications
- Fits the power user requirements – customization of the mechanism reduction and analysis Interactive Model explorer for building a workflow of mechanism reduction, Wide set of reduction targets, Multi-target multi-point reduction of kinetic mechanisms
- Seamless integration with existing computational infrastructure – supports widely accepted kinetic mechanism file formats for direct import into engineering analysis software (CFD)

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