# COMSOL RELEASE NOTES

VERSION 4.0a



#### Benelux

COMSOL BV
Röntgenlaan 19
2719 DX Zoetermeer
The Netherlands
Phone: +31 (0) 79 363 4230
Fax: +31 (0) 79 361 4212
info@comsol.nl
www.comsol.nl

#### Denmark

COMSOL A/S Diplomvej 376 2800 Kgs. Lyngby Phone: +45 88 70 82 00 Fare: +45 88 70 80 90 info@comsol.dk www.comsol.dk

#### Finland

COMSOL OY Arabiankatu 12 FIN-00560 Helsinki Phone: +358 9 2510 400 Fax: +358 9 2510 4010 info@comsol.fi www.comsol.fi

#### France

COMSOL France WTC, 5 pl. Robert Schuman F-38000 Grenoble Phone: +33 (0)4 76 46 49 01 Fax: +33 (0)4 76 46 07 42 info@comsol.fr www.comsol.fr

#### Germany

COMSOL Multiphysics GmbH Berliner Str. 4 D-37073 Göttingen Phone: +49-551-99721-0 Fax: +49-551-99721-29 info@comsol.de www.comsol.de

#### India

COMSOL Multiphysics Pvt. Ltd. Esquire Centre C-Block, 3rd Floor No. 9, M. G. Road Bangalore 560001 Karnataka Phone: +91-80-4092-3859 Fax: +91-80-4092-3856 info@comsol.co.in

#### Italy

COMSOL S.r.l. Via Vittorio Emanuele II, 22 25122 Brescia Phone: +39-030-3793800 Fax: +39-030-3793899 info.it@comsol.com www.it.comsol.com

#### Norway

COMSOL AS Søndre gate 7 NO-7485 Trondheim Phone: +47 73 84 24 00 Fax: +47 73 84 24 01 info@comsol.no www.comsol.no

### Sweden

COMSOL AB
Tegnérgatan 23
SE-111 40 Stockholm
Phone: +46 8 412 95 00
Fax: +46 8 412 95 10
info@comsol.se
www.comsol.se

#### Switzerland

COMSOL Multiphysics GmbH Technoparkstrasse I CH-8005 Zürich Phone: +41 (0)44 445 2140 Fax: +41 (0)44 445 2141 info@ch.comsol.com www.ch.comsol.com

#### United Kingdom COMSOL Ltd.

UH Innovation Centre College Lane Hatfield Hertfordshire AL10 9AB Phone: +44-(0)-1707 636020 Fax: +44-(0)-1707 284746 info.uk@comsol.com www.uk.comsol.com

#### **United States**

COMSOL, Inc.
I New England Executive Park
Suite 350
Burlington, MA 01803
Phone: +1-781-273-3322
Fax: +1-781-273-6603

COMSOL, Inc. 10850 Wilshire Boulevard Suite 800 Los Angeles, CA 90024 Phone: +1-310-441-4800 Fax: +1-310-441-0868

COMSOL, Inc. 744 Cowper Street Palo Alto, CA 94301 Phone: +1-650-324-9935 Fax: +1-650-324-9936

info@comsol.com www.comsol.com

For a complete list of international representatives, visit www.comsol.com/contact

# Company home page www.comsol.com

COMSOL user forums www.comsol.com/support/forums

#### COMSOL Release Notes

© COPYRIGHT 1998-2010 COMSOL AB.

Protected by U.S. Patents 7,519,518; 7,596,474; and 7,623,991. Patents pending.

The software described in this document is furnished under a license agreement. The software may be used or copied only under the terms of the license agreement. No part of this manual may be photocopied or reproduced in any form without prior written consent from COMSOL AB.

COMSOL and COMSOL Multiphysics are registered trademarks of COMSOL AB. LiveLink and COMSOL Desktop are trademarks of COMSOL AB..

Other product or brand names are trademarks or registered trademarks of their respective holders.

Version: June 2010 COMSOL 4.0a

Part number: CM010001

# Release Notes

COMSOL Multiphysics version 4.0a is in many aspects an entirely new product. This document outlines the differences between version 3.5a and version 4.0a. It also outlines additions that we plan to make in COMSOL Multiphysics version 4.1.

We have strived to achieve backward compatibility with the previous version and to include all functionality that is available there. COMSOL 4.0a is compatible with COMSOL 3.5a and COMSOL 4.0 with some exceptions. Those exceptions are noted in this document.

# COMSOL Multiphysics

COMSOL Multiphysics version 4 introduces many new ideas and concepts making it easier for you to create models. The following lists the most important updates to the graphical user interface.

**New layout:** In version 4 it is easier to organize and design models with the intuitive structure of the COMSOL Desktop. The Model Builder displays all the features of your model in one place.

**Personalized desktop:** Control how you organize the COMSOL Desktop layout—your preferences are saved for the next time you open COMSOL Multiphysics.

**Sequences of operations:** You can now build custom model sequences to generate your geometry, physics, mesh, studies, and results. The sequences can be edited and changes are automatically updated across the model. Operations in the sequences can be modified by the parametric solver.

Geometric parameter sweeps: With geometry sequences COMSOL can perform geometric parameter sweeps with full associativity from the user interface.

Material settings: Materials are now administrated in one node in the Model Builder. You can select a material and its properties for each domain and for all physics in that domain.

**Multiple solutions and meshes:** With the new layout, you can save and view multiple solutions and meshes, and compare and contrast the results in the *Results* branch.

**Probes:** Use probes to visualize scalar quantities during computations. The quantities can be defined as integrals, max/min, the average of a field quantity, or the value at a point. This now works for time stepping and parameter sweeps.

**Dynamic help:** The new context-dependent help enables easy browsing with extended search functionality. The Help Menu provides access to the complete documentation set in PDF and HTML formats.

**Improved graphics:** Faster, better looking graphics.

**Model settings:** Access to the model settings is easier and more intuitive. When you select a node in the Model Builder, a docked window containing associated settings displays at the same time.

**Predefined selections:** Define selections of domains, boundaries, edges, and points. These predefined selections are available in the Settings windows for the physics interfaces, meshing, and when studying the results.

LiveLink™ family of products for integrating with CAD and MATLAB® The new LiveLink<sup>™</sup> for SolidWorks®, LiveLink<sup>™</sup> for Inventor®, and LiveLink<sup>™</sup> for Pro/ ENGINEER® products connect COMSOL Multiphysics directly with these CAD programs for interactively linking parameters specified in a CAD system with simulation geometry. In addition, LiveLink for MATLAB is available for incorporating COMSOL Multiphysics models in the MATLAB technical computing and programming environment.

**Cluster support** A floating network license for COMSOL Multiphysics can be extended at no additional cost to computational nodes for clusters on the Windows Cluster Server 2003, Windows HPC Server 2008, and Linux platforms.

## Version 4 also introduces:

- New and enhanced physics interfaces and predefined multiphysics interfaces
- New parallel solvers and higher solver performance:
  - A modal solver for frequency response and time domain (for structural and acoustics simulations, for example)
  - The MUMPS and SPOOLES direct solvers for parallel and cluster computing
  - A time discrete solver
  - A fast-frequency sweep solver using AWE (asymptotic waveform evaluation) for electromagnetic waves simulations, for example

# New Modules in Version 4.0a

# COMSOL Multiphysics 4.0a includes four new modules:

• CFD Module: for modeling laminar and turbulent single-phase and multiphase fluid flow, conjugate heat transfer, porous media flow, thin-film flow and lubrication, and other applications within fluid dynamics.

- Batteries and Fuel Cells Module: for modeling batteries, fuel cells, and other electrochemical applications.
- Plasma Module: for modeling plasma physics such as inductively-coupled and capacitively-coupled plasma, microwave plasma, drift-diffusion processes, and heavy species transport.
- Chemical Reaction Engineering Module: For modeling chemical reactions and chemical species transport using both space-dependent and space-independent models. The chemical reactions can be coupled to heat transfer and fluid flow. This module replaces the Chemical Engineering Module and the Reaction Engineering Module in 4.0 (see "Backward Compatibility vs. Version 4.0" below).

Backward Compatibility vs. Version 4.0

#### CHEMICAL ENGINEERING AND REACTION ENGINEERING MODULES

COSMOL Multiphysics 4.0a introduces the new Chemical Reaction Engineering Module, which merges the Chemical Engineering Module and the Reaction Engineering Module. All the reaction engineering tools are now integrated with the chemical species transport tools in the same module. The Chemical Reaction Engineering Module is focused on reaction engineering and chemical species transport and for that reason excludes many of the fluid flow capabilities of the former Chemical Engineering Module. Those fluid flow capabilities are instead included in the new CFD Module.

# CHANGED DEFAULT ELEMENT ORDER FOR SOME PHYSICS INTERFACES

Many of the transport interfaces for fluid flow, heat transfer, and chemical species transport now use first-order elements (shape functions) by default instead of second-order elements which was the default in version 4.0. The reason for this is that higher-order elements are computationally more costly than linear elements, and also more prone to introduce spurious oscillations, which reduces the numerical robustness.

For the following physics interfaces, the default element order has changed:

- The Laminar Flow and Turbulent Flow single-phase flow interfaces uses linear elements for both the velocity field and the pressure (P1 + P1 elements).
- The Phase-Field Two-Phase Flow interface uses linear elements for both the velocity field and the pressure (P1 + P1 elements).

- Heat Transfer in Fluids and Heat Transfer in Porous Media use linear elements for the temperature.
- All interfaces in the Chemical Species Transport branch (Transport of Diluted Species, Transport of Concentrated Species, Nernst-Planck Equations, Solute Transport, and Species Transport in Porous Media) use linear elements for the species concentrations.
- In the Fluid-Structure Interaction interface you can control the element order for the structural mechanics and the fluid flow separately. The default uses second-order elements for the displacements in the structure and linear elements for the velocity field and pressure in the fluid.
- The Non-Isothermal Flow and Conjugate Heat Transfer interfaces use the same element order for the temperature as for the velocity field. The default setting uses linear elements for the temperature and the velocity field.
- In the Thermal Stress interface the element order for the temperature is one order lower than for the displacements. The default setting uses second-order elements for the displacements and linear elements for the temperature.

With the new default element orders, it can still be beneficial to use second-order elements rather than the default linear elements in the following cases:

- Laminar Flow for low flow velocities.
- Phase-Field Two-Phase Flow for microfluidics applications where convection is
- Heat Transfer in Participating Media for cases when the media is approximated as stationary.
- Heat Transfer in Porous Media when convection is negligible.
- Chemical Transport interfaces when simulating only diffusion.

In these cases, increasing the element order is an effective alternative to refining the mesh.

**Note:** The changed default settings do not affect models created using version 4.0.

#### DEFORMED GEOMETRY INTERFACE

The Parameterized Geometry application mode in versions 3.5a, which is limited to 2D, is replaced with the Deformed Geometry interface in version 4.0a. This interface is available in 2D and 3D. The *Deformed Geometry* interface deforms the mesh using an arbitrary Lagrangian-Eulerian (ALE) method and is not the parameterized geometry using geometric parameter sweeps (see above), which is new functionality in version 4.0a.

In the version 4.0a interface, the *Linear Displacement* and *Similarity Transform* boundary conditions are not yet available as preset conditions. Those boundary conditions are planned for version 4.1.

In version 4.0a, you can create the corresponding conditions by manually entering variables.

#### PAIR BOUNDARY CONDITIONS

Pairs are used to connect boundaries between domains that are separated by an assembly boundary (boundary between different parts in an assembly). To create an assembly, you have to either import it from a CAD package or actively form an assembly as a final step in the COMSOL geometry sequence.

Pair boundary conditions are available as general conditions for all application modes in versions 3.5a. Most pair boundary conditions that were available in COMSOL 3.5a can be found in the physics interfaces in version 4.0a. Exceptions from this are listed under backward compatibility for each product.

# PERIODIC PAIR BOUNDARY CONDITIONS

Periodic boundary conditions are used to model repetitive structures, where one boundary in a domain is identical to another boundary in the same domain.

Periodic boundary conditions are available as general conditions for all application modes (now called physics interfaces) in version 3.5a. In version 4.0, this functionality is a tailored condition for each physics interface.

However, some physics interfaces may lack periodic boundary conditions in version 4.0; see the *Backwards Compatibility* section for the modules below.

Note that, in the future, all physics interfaces will include periodic boundary conditions.

#### PDE MODES

Basis Functions or Elements

The PDE application mode in version 3.5a includes a number of possible basis functions or elements to be used in the finite element formulation of a set of equations.

Only Lagrange basis elements are available in the PDE interfaces in version 4.0a using the General form or Coefficient form. Discontinuous elements are available by entering expressions as weak contributions using auxiliary dependent variables.

Other elements are not yet available in the PDE interfaces.

#### **WEAK CONSTRAINTS**

There are some physics interfaces that are not able to define constraints as weak constraints; see the Backwards Compatibility sections for the modules below.

## **AXISYMMETRIC MODELS**

In version 3.5a equations in axisymmetric application modes use the *independent* variable for the radius, r, to account for axisymmetry. In version 4.0a, the equations are compensated by using the factor  $2\pi r$ .

**Note:** If you have manually multiplied expressions by  $2\pi$  for a version 3.5a model, these may be incorrect when the model is opened in version 4.0a.

# DISPLAY OF EQUATIONS

The equations for the physics interfaces are not displayed graphically in version 4.0a. However, using dynamic help, you can get an overview of the equations formulated by a physics interface by just one click. Full support for display of equations is planned for version 4.1.

## REPORT GENERATOR

The report generator is not yet implemented in version 4.0a. A report generator is planned for 4.1.

# BACKWARD COMPATIBILITY FOR PRE-3.5A MODELS

COMSOL 4.0a can load models saved from version 3.5a. For loading models from earlier COMSOL versions than 3.5a you need to load them in COMSOL 3.5a and then save them. For simplifying this task a utility is available where you can convert all

files in a directory from versions 3.0-3.5 to version 3.5a. See the section "COMSOL Convertpre35a Command" on page 43 for Windows, section "COMSOL Convertpre35a Command" on page 76 for Linux, section "COMSOL Convertpre35a Command" on page 101 for the Mac in the COMSOL Installation and Operations Guide for more information.

# AC/DC Module

# New Functionality in Version 4

This release of the AC/DC Module includes a number of new capabilities. Some of the most important ones are the following:

- Electric and magnetic point dipoles allow for easy and computationally efficient modeling of electromagnetic sources. Many coils and electrostatic applications can be approximated by one or more point dipoles.
- The Transition boundary condition for metallic layers of arbitrary thickness provides accurate modeling of geometrically thin metal sheets without having to mesh the thickness. This substantially helps to reduce the number of elements and the problem size. The layer can be of arbitrary electrical thickness (measured relative to the skin depth) and have a more or less pronounced discontinuity in the tangential electric field.
- The Contact Resistance boundary condition for efficient modeling of thin resistive sheets provides accurate modeling of geometrically thin highly resistive sheets without having to mesh the thickness. This substantially helps to reduce the number of elements and the problem size. The type of layer modeled using the contact resistance condition typically has a discontinuity in the normal electric field.
- Discontinuous interior boundary conditions like electric insulation for electric currents and perfect magnetic conductor for magnetic fields are now available.
- Single-turn coil domain and multi-turn coil domain modeling in 2D allow for easy modeling of coil domains in 2D and also support connection to electrical circuits (integrated with the new Electrical Circuit interface, described below). One or more geometrical domains can be assigned as voltage or current-driven coil. More than one geometrical domain can be treated as belonging to the same coil. This functionality replaces the use of manual model couplings in previous versions.
- The new *Electrical Circuit* physics interface with predefined passive and active components is integrated with all the other interfaces in the AC/DC Module via the terminal boundary condition and the single-turn and multi-turn coil domain functionality. It is now possible to build electrical circuits directly in the Model Builder. SPICE netlists are imported and translated into native and editable COMSOL circuit elements in the Model Builder.

- A new moving mesh interface for *rotating machinery* is now implemented in version 4.0 where the Moving Mesh (ALE) physics interface is much easier to use compared to previous versions. You can use this interface to implement new rotating machinery models. For backward compatibility for old rotating machinery models, see below.
- Port/Terminal sweep for frequency-dependent lumped parameter calculations in the graphical user interface makes it easy to compute full lumped parameter matrices. These can be exported in the text-based Touchstone file format.

Backward Compatibility vs. Version 3.5a

## CHANGE IN DEPENDENT VARIABLES

Version 4 has a comprehensive set of inductive formulations based on the magnetic vector potential. These cover all modeling situations except for situations with strongly nonlinear conductivity (superconductors) for which magnetic field H-based formulations are more suitable.

The 2D formulations based on the magnetic field H as dependent variable in version 3.5a are not yet included in version 4.0. A full set (3D, 2D and 2D axisymmetry) of Hbased formulations is planned for version 4.1.

Models created in version 3.5a that are built using an H based formulation will not include any physics interface settings when opened in version 4.0. Geometrical data and definitions (constants and expressions) will be imported and the physics can manually be added using the (vector potential based) Magnetic Fields interface.

## PAIR BOUNDARY CONDITIONS

The Contact Resistance, Transition, and Perfect Magnetic Conductor boundary conditions are not yet available as assembly Pair boundary conditions.

A new set of slit-based, discontinuous boundary conditions, which does not require assemblies is introduced in version 4. In most models, this can replace the assembly pair boundary condition.

# Acoustics Module

# New Functionality in Version 4

- The definition of material properties has been reworked and extended, both for frequency and time domains.
- Thin interior walls—hard, with acceleration, impedance or perforations—can now be defined directly as boundary conditions. No modification to the geometry is necessary.
- The Scattered field formulation no longer makes any assumptions about the incident field. This makes it easier to model complicated situations with both fluid-fluid and fluid-solid interfaces.
- A new multiphysics interface for acoustic-structure interaction has been added. The coupling between fluids and solids is fully automated.

# Backward Compatibility

# ULTRAWEAK FORMULATION

The *ultraweak formulation* is not implemented in version 4.0a and is not planned for re-implementation in its previous form. The reason is that this formulation is very difficult to use without basis element order adaptivity (p-adaptivity).

## PAIR BOUNDARY CONDITIONS

Vortex sheet condition on assembly pair boundaries is missing in the Aeroacoustics interface. You can use the slit-based vortex sheet boundary condition instead.

# CFD Module

This section described new functionality and backward compatibility with respect to the implementations in the Chemical Engineering Module in COMSOL 3.5a.

# New Functionality in Version 4

- A new Low-Reynolds Number k-& Turbulence Model interface is introduced, which yields high accuracy in the description of the flow close to walls. Mass and heat transport are also accurately described by this formulation.
- The improved k- $\varepsilon$  *Turbulence Model* interface implementation gives greater robustness when the value of the turbulence intensity is small. The wall functions are also more accurate and require less input compared to previous versions.
- The new turbulence model formulations allow for transient simulations of turbulent flow. You can run time-dependent simulations without having to start with a steady flow solution as initial condition.
- The option to use psuedo time stepping when computing stationary solutions has been added to the Single-Phase Flow physics interfaces (including Brinkman Equations and Free and Porous Media Flow). Pseudo-time stepping increases the robustness when solving highly non-linear problems and reduces the need for solving in several steps.
- The multiphysics interface Rotating Machinery has been substantially improved. Using the Rotating Domain feature one or several rotating domains can be included in a model. The axis of rotation can easily be altered as well as the rotation direction and frequency. The Rotating Wall feature automatically adds the proper velocity constraints on boundaries of the Rotating Domain feature which do not correspond to the interface between the rotating and stationary domain.
- The possibility to include a Forchheimer Drag extension to the fluid flow resistance in porous media flow has been added.
- It is now possible to include a convective term in the Brinkman Equations. This means that porous media flow including higher fluid velocity can be studied. The inclusion of the term is controlled using the Neglect inertial term (Stokes-Brinkman) switch available in the Brinkman Equations and the Free and Porous Media physics interfaces.

- Stabilization has been included for the Brinkman equations. The stabilization provides increased robustness and less computational cost for a given accuracy compared to previous versions. It is also imperative when solving problems including the convective term.
- You can now add and remove species in the *Chemical Species Transport* interfaces. This means that you do not have to start with all species in your transport model. Instead you can add species one by one, thus reducing the risks for introducing errors.
- Two new diffusion models, a mixture-averaged diffusion model and a model based on Fick's law, are introduced in the Transport of Concentrated Species interface. These diffusion models are less computationally demanding than the Maxwell-Stefan diffusion model, and the latter model require less input data for the interaction between species in the mixture. The new models can be used in convectively dominated problems, where high accuracy in the diffusion interaction is not required, or when interaction data is not available.
- The improved stabilization for *Chemical Species Transport* in version 4.0 yields higher accuracy with a relatively coarse mesh compared to version 3.5a. This also results in increased robustness and less computational cost for a given accuracy compared to previous versions.
- A new *Open Boundary* condition is introduced in the physics interfaces for turbulent Single Phase Flow, Heat Transfer, and Chemical Species Transport. The condition is designed to be used on model boundaries including both in and outflow sections. On sections with inflow the solution is not affected, while at occurrences of inflow a user defined exterior condition is enforced.
- A new physics interface for Species Transport in Porous Media accounts for the effect of the tortuous path in porous media. This path results in the additional dispersion perpendicular to the main flow of a transported species caused by the convective flux. The dispersion of species in porous media is thus more accurately described compared to previous implementations.
- A new physics interface for Heat Transfer in Porous Media can be used to accurately study heat transfer in porous catalysts, filters, and other unit operations involving porous media.

#### **K-ε TURBULENCE MODEL**

The new wall functions have the potential to deliver higher accuracy than the formulation used in 3.5a. They may however require finer wall resolution. Hence, a 3.5a turbulence model can often benefit from an additional boundary layer mesh or refined boundary layer mesh when imported into 4.0a.

## K-ω TURBULENCE MODEL

The k- $\omega$  turbulence model physics interface is not yet implemented in version 4.0a. It is planned for the CFD Module in version 4.1.

Version 4.0a includes automatic translation of models built with the previous  $k-\omega$ turbulence model. When opened, the full model, including initial values and boundary conditions, is converted to the k- $\epsilon$  turbulence model. Once opened, the model can also be also be changed to the Low-Reynolds k-e Turbulence Model interface. The latter physics interface present an excellent alternative for higher accuracy in models including confined flows.

## PSEUDO APPLICATION MODES

The Pseudo application modes for species transport in version 3.5a allow for the use of the dependent variable for time as a space coordinate in the direction of the flow.

The corresponding physics interfaces are not yet implemented in version 4.0a. They are planned for a later version.

Meanwhile, you can either create this alternative description manually, by relating time to a position along the length of the reactor using the axial velocity, or you can use a full 2D or 3D model.

#### SPECIAL BASIS FUNCTIONS OR ELEMENTS

None of the special basis functions or elements for the finite element formulation of flow problems included in version 3.5a are available in version 4.0a. However, the new stabilization functionality in version 4.0a for fluid flow is identical to using the bubble elements in 3.5a.

Other special elements that were available in 3.5a will not be re-implemented in version 4. The reason for this is that the stabilized formulation in version 4.0a gives high accuracy to a relatively small computational cost compared to the special elements.

# THIN BOUNDARY LAYER PAIR BOUNDARY CONDITIONS

The thin boundary layer approximation approximates the mass flux perpendicular to an interface according to:

$$\mathbf{n}_i \cdot \mathbf{n} = -k(c_b - c_s)$$

where  $\mathbf{n}_i$  denotes the flux of species i,  $\mathbf{n}$  the normal vector,  $c_s$  the surface concentration, and  $c_b$  the bulk concentration of species i.

In the case where  $c_s$  actually is a concentration in a separate domain, so that the interface between two domains requires a discontinuous concentration but a continuous flux, this condition could be defined in 3.5a using pair boundary conditions.

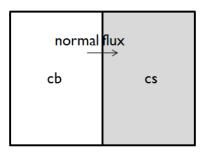


Figure 1-1: Example of two domains with two separate dependent variables for chemical

Version 3.5a models using this functionality are not automatically converted to version 4.0a.

However, you can covert these models manually in version 4.0a by using separate fields for the surface and bulk concentrations. The analogy is also valid for heat flux.

# Chemical Reaction Engineering Module

# New Functionality in Version 4

- You can now add and remove species in the Chemical Species Transport physics interfaces. This means that you do not have to start with all species in your transport model. Instead you can add species one by one, thus reducing the risks for introducing errors.
- Two new diffusion models, a mixture-averaged diffusion model and a model based on Fick's law, are introduced in the Transport of Concentrated Species interface. These diffusion models are less computationally demanding than the Maxwell-Stefan diffusion model, and the latter model require less input data for the interaction between species in the mixture. The new models can be used in convection dominated problems, where high accuracy in the diffusion interaction is not required, or when interaction data is not available.
- The improved stabilization for *Chemical Species Transport* in version 4 yields higher accuracy with a relatively coarse mesh compared to version 3.5a. This also results in increased robustness and less computational cost for a given accuracy compared to previous versions.
- The possibility to include a *Forchheimer Drag* extension to the fluid flow resistance in porous media flow has been added.
- It is now possible to include a convective term in the Brinkman Equations. This means that porous media flow including higher fluid velocity can be studied. The inclusion of the term is controlled using the Neglect inertial term (Stokes-Brinkman) switch available in the Brinkman Equations and the Free and Porous Media physics interfaces.
- Stabilization has been included for the Brinkman equations. The stabilization provides increased robustness and less computational cost for a given accuracy compared to previous versions. It is also imperative when solving problems including the convective term.
- A new Open Boundary condition is introduced in the physics interfaces for chemical species transport. The condition is designed to be used on model boundaries including both convective in and outflow sections. On sections with inflow the

species concentration is not affected, while on sections with inflow a user defined exterior concentration is enforced.

- A new physics interface for Species Transport in Porous Media accounts for the effect of the tortuous path in porous media. This path results in the additional dispersion perpendicular to the main flow of a transported species caused by the convective flux. The dispersion of species in porous media is thus more accurately described compared to previous implementations.
- A new physics interface for *Heat Transfer in Porous Media* can be used to accurately study heat transfer in porous catalysts, filters, and other unit operations involving porous media.

Backward Compatibility vs. Version 3.5a

#### **PSEUDO APPLICATION MODES**

The Pseudo application modes for species transport in version 3.5a allow for the use of the dependent variable for time as a space coordinate in the direction of the flow.

The corresponding physics interfaces are not yet implemented in version 4.0a. They are planned for 4.1.

Meanwhile, you can either create this alternative description manually, by relating time to a position along the length of the reactor using the axial velocity, or you can use a full 2D or 3D model.

# THIN BOUNDARY LAYER PAIR BOUNDARY CONDITIONS

The thin boundary layer approximation approximates the mass flux perpendicular to an interface according to:

$$\mathbf{n}_i \cdot \mathbf{n} = -k(c_b - c_s)$$

where  $\mathbf{n}_i$  denotes the flux of species i,  $\mathbf{n}$  the normal vector,  $c_s$  the surface concentration, and  $c_b$  the bulk concentration of species i.

In the case where  $c_s$  actually is a concentration in a separate domain, so that the interface between two domains requires a discontinuous concentration but a continuous flux, this condition could be defined in 3.5a using pair boundary conditions.

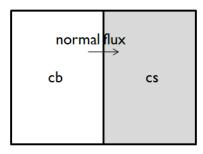


Figure 1-2: Example of two domains with two separate dependent variables for chemical concentration.

Version 3.5a models using this functionality are not automatically converted to version 4.0a.

However, you can covert these models manually in version 4.0a by using separate fields for the surface and bulk concentrations. The analogy is also valid for heat flux.

# EQUILIBRIUM REACTIONS AND MASS TRANSPORT

The equilibrium reaction assumptions defined by entering in the Reaction Engineering interface does not automatically generate space-dependent formulations. This functionality will be implemented in a later version.

# Earth Science Module

# New Functionality in Version 4

- The physics interface for *Heat Transfer in Porous Media* now accounts for multiple immobile solids and fluids. There are two choices for averaging the thermal conductivity: volume average and a power law formulation.
- The physics interface for Heat Transfer in Porous Media also incorporates options for describing geothermal heating and thermal dispersion.
- The previous three separate formulations of *Darcy's law* (pressure, pressure head, and hydraulic head) are available in one framework in version 4.0a. This makes it possible to mix boundary and initial conditions using any of these formulations. The Porous Media and Subsurface Flow physics interfaces are also able to specify isotropic, orthotropic or anisotropic permeabilities or hydraulic conductivities.
- The physics interface for *Poroelasticity* includes a poroelastic material model to account for isotropic poroelastic materials. The material properties can be written in terms of bulk and shear modulus, Young's modulus and Poisson ratio, Lamé constants, or pressure and shear velocities. Orthotropic and fully anisotropic materials can be modeled if used together to the SME module.
- A new physics interface for *Solute Transport* incorporates the old application modes for solute transport in saturated porous media and variable saturated porous media in one physics interface. You can also add and remove species freely in the Chemical Species Transport physics interfaces.
- A new physics interface for Fracture Flow enables the solution of Darcy's Law in thin shells and fractures, without having to mesh along the thickness of a thin layer. This substantially improves performance for a given accuracy compared to previous versions.
- You can specify the *unit of time* in days and years in the time-dependent solver. This improves the usability for geotechnical processes compared to the use of seconds.
- Darcy's Law can now handle variable densities.
- The possibility to include a Forchheimer Drag extension to the fluid flow resistance in porous media flow has been added.
- It is now possible to include a convective term in the Brinkman Equations. This means that porous media flow including higher fluid velocity can be studied. The inclusion of the term is controlled using the Neglect inertial term

(Stokes-Brinkman) switch available in the Brinkman Equations and the Free and Porous Media physics interfaces.

• Stabilization has been included for the Brinkman equations. The stabilization provides increased robustness and less computational cost for a given accuracy compared to previous versions. It is also imperative when solving problems including the convective term.

Backward Compatibility vs. Version 3.5a

## SPECIAL BASIS FUNCTIONS OR ELEMENTS

None of the special basis functions or elements for the finite element formulation of flow problems featured in version 3.5a are available in version 4.0a. However, the new stabilization functionality in version 4.0a for fluid flow is identical to using the bubble elements in 3.5a.

Other special elements that were available in 3.5a will not be re-implemented in version 4. The reason for this is that the stabilized formulation in version 4.0a gives high accuracy to a relatively small computational cost compared to the special elements.

# Heat Transfer Module

# New Functionality in Version 4

- A new Conjugate Heat Transfer multiphysics interface (fluid flow, fluid heat transfer, and solid heat transfer) for modeling electronic cooling and heat sinks, for example.
- A new physics interface for Heat Transfer in Porous Media accounts for the effect of a tortuous path, which results in the additional convective thermal dispersion perpendicular to the main flow. The temperature field is thus more accurately described compared to previous implementations.
- A new physics interface for Radiation in Participating Media introduces the effect of absorption of energy in a media subjected to radiation. The radiation pattern from one surface to another then depends on the media present between the radiating or reflecting surfaces.
- The new physics interface for Low-Reynolds Number k-& Turbulence Model yields a higher accuracy in the description of the flow and heat transfer close to walls.
- The new *Open Boundary* condition is useful for modeling an open boundary where heat can flow out from the domain or into the domain with a specified exterior temperature.
- Improved stabilization yields increased robustness and higher accuracy for a given computational cost compared to previous versions.

# Backward Compatibility vs. 3.5a

## **K-ε TURBULENCE MODEL**

The new wall functions have the potential to deliver higher accuracy than the formulation used in 3.5a. They may however require finer wall resolution. Hence, a 3.5a turbulence model can often benefit from an additional boundary layer mesh or refined boundary layer mesh when imported into 4.0a.

#### K-ω TURBULENCE MODEL

The k- $\omega$  turbulence model physics interface is not yet implemented in version 4.0a. It is planned for the CFD Module in version 4.1.

Version 4.0a includes automatic translation of models built with the previous  $k-\omega$ turbulence model. When opened, the full model including initial values and boundary conditions, is converted into using the k- $\epsilon$  turbulence model. Once opened the model can also be also be changed into using the Low-Reynolds k-e turbulence model interface. The latter interface present an excellent alternative for higher accuracy in models including confined flows.

# TURBULENT FLOW WITH WALL FUNCTIONS AND HEAT TRANSFER IN CONJUGATE HEAT TRANSFER

Highly conductive layers on the interface between a solid and a fluid are not yet fully implemented and give incorrect results when used in combination with wall functions in turbulent flow. This is caused by the incorrect definition of the wall temperature as the average of the solid and fluid temperature in these physics interfaces.

In some case, you can correct this in equation view. Please contact technical support if you run into problems with such a model.

Momentum transport Wall Functions are translated into the revised Wall Functions in 4.0a. The Heat equation Wall Functions are also translated, but the translated formulation uses the default turbulence modeling constants, regardless of the values that were defined in Physics>Scalar Variables in 3.5a.

# SURFACE-TO-SURFACE RADIATION IN COMBINATION WITH TURBULENT FLOW AND HEAT TRANSFER

It is currently not possible to include surface-to-surface radiation in models using the coupled turbulent flow and heat transfer interfaces. The reason for this is that the wall temperature is incorrectly defined as the average of the fluid temperature and the solid temperature in version 4.0a.

# MEMS Module

# New Functionality in Version 4

- New physics interfaces are added for Thin-Film Flow and Thin-Film Gas Flow (using a conventional and modified Reynolds equation, respectively). These allow you to account for the influence of thin squeezed films that also include a substantial effect from a flow that runs in parallel to the squeezing surfaces in 2D models.
- A new Lubrication Shell interface for modeling lubrication by thin fluid films in narrow geometries that can be represented as shells. This gives high accuracy at a much smaller computational cost compared to full fluid-structure interaction in 3D with moving boundaries.
- Version 4 also includes an improved physics interface for *Piezoelectric Devices*. This new interface gives full access to the functionality of the structural mechanics and electrostatics physics interfaces in addition to the piezoelectric material model.

# Backward Compatibility

## PIEZOELECTRIC DEVICES INTERFACE

The following 3.5a functionality is not available in version 4.0a:

- Electrical formulations
- Initial electric displacement

## FILM DAMPING

- The solid predefined coupling is missing but can be performed manually
- Perforated plates are not yet available. These have to be modeled in version 4.0a using the full geometric description or using equation view.

# RF Module

# New Functionality in Version 4

- Electric and magnetic point dipoles allow for easy and computationally efficient incorporation of electromagnetic sources in electromagnetic wave propagation models. Many antennas can be approximated by one or more point dipoles.
- A Transition boundary condition for metallic layers of arbitrary thickness provides accurate modeling of geometrically thin metal sheets without having to mesh the thickness. This substantially helps to reduce the number of elements and the problem size. The layer can be of arbitrary electrical thickness (measured relative to the skin depth) and have a more or less pronounced discontinuity in the tangential electric field.
- The discontinuous interior boundary condition perfect magnetic conductor is now
- A new variational S-parameter formulation supports multimode ports and numerical hybrid-mode ports. This allows for accurate modeling of dielectrically loaded waveguides and optical waveguides.
- Port sweep for frequency-dependent S-parameter calculations in the graphical user interface makes it easy to compute full S-parameter matrices. These can be exported in the Touchstone file format.
- The new *Electrical Circuit* physics interface with predefined passive and active components is integrated with other physics interfaces in the RF Module via the port and lumped port boundary conditions. It is now possible to build electrical circuits directly in the Model Builder. SPICE netlists are imported and translated into native and editable COMSOL circuit elements in the Model Builder.

Backward Compatibility vs Version 3.5a

#### CHANGE IN DEPENDENT VARIABLES

Version 4.0a has a comprehensive set of electromagnetic wave propagation formulations based on the electric field that covers all modeling situations.

However, it is no longer possible to solve for the magnetic field H as a dependent variable.

Models saved in version 3.5a that are based on an H formulation are translated to the new E formulation but need to be solved again to update the solution in version 4.0.

# FAR-FIELD POSTPROCESSING

Far fields are not automatically read in when importing a 3.5a model into version 4.0a. The workaround is to manually add a Far Field Calculation node.

## PAIR BOUNDARY CONDITIONS

Pair boundary conditions are not yet implemented, except for some basic features.

This means that the assembly port boundary condition is not supported in version 4.0.

# Reaction Engineering Module

See the Section "Chemical Reaction Engineering Module" on page 16. The reaction engineering module has been merged with the Chemical Engineering Module from 4.0.

# Structural Mechanics Module

# New Functionality for Version 4

- A flexible definition of elastic material data enables the solid mechanics interfaces to support bulk modulus and shear modulus, Lamé constants, and pressure-wave and shear-wave speed in addition to Young's modulus and Poisson's ratio.
- Custom hyperelastic material models can be created by specifying a strain energy function in terms of deformation tensor components and invariants.
- A flexible 2D solid mechanics interface allows you to switch between plane stress and plane strain approximations at any point during modeling. For example, it is now easy to compare the results with plane strain and plane stress assumptions.
- Prescribed velocity and acceleration boundary conditions are now available also in transient analysis. Previously, these conditions were available only in the frequency domain.
- A new rigid connector boundary condition (only in 3D in version 4.0) makes it possible to apply kinematic constraints, forces, and moments on boundaries assumed to displace as a rigid body.
- A new 3D shell and 2D plate element formulations based on first-order or second-order Lagrange shape functions on both triangles and quadrilaterals gives improved accuracy. Curved surfaces and mixed solid-shell models, in particular, are improved. In addition, the new shell elements are fully multiphysics-enabled and support large deformations and anisotropic materials.
- Frequency-domain and time-domain *modal solvers* let you run fast frequency sweeps and transient response analyses on reduced models.
- The *Elastoplastic Material Model* now allows the use of a non associated flow rule.

# Backward Compatibility

# **CROSS-SECTION LIBRARY**

The cross-section library for beams is not available in version 4.0a. This is planned for version 4.1.

#### PLANE STRESS

Version 4 represents the out-of-plane strain as a separate degree of freedom. Plane stress models made with version 3.5a need to be re-solved to correctly compute strains and stresses. Displacements are correctly computed.

#### SYMBOLS

Symbols in the graphics window representing constraints and loads are not yet available in version 4.0a. Symbols will be available in version 4.1.

## ITERATIVE SOLVER USED IN 3D BY DEFAULT

GMRES/GMG with LU preconditioner is the default solver in version 4.0a for 3D static and time dependent studies.

For stretched elements, this solver may run into convergence problems. If you run into convergence problems, try to improve the quality of the tetrahedral mesh by reducing the variations in mesh size. For smaller and medium-size problems, switch to a direct solver.

# LiveLink for MATLAB

# New Functionality

The model object that contains the true representation of the model is available directly from the MATLAB® prompt. This means that all functionality available from the COMSOL Desktop becomes automatically available at the MATLAB prompt, and that the model behaves exactly the same from the MATLAB prompt as it does in the COMSOL Desktop. In the future this will also mean that you will be able to see changes to the model object that have been made in MATLAB, and vice versa.

The interface to MATLAB uses an entirely new syntax for the model. In order to help you convert models to the new syntax, two conversion tools are available:

- The function mphv4
- The ability to load 3.5a models in the V4 GUI and then to save them as M-files

These conversion tools are limited to converting the fem structure to the new syntax; the rest of the M-files that you have written for 3.5a need to be manually converted.

The ability to start COMSOL with MATLAB in a 3.5a compatibility mode is intended to help you in the process of working with both the old and new syntax.

## Parameterized Geometries

Version 4.0a includes built-in support for parameterized geometries. There should be no need to change boundary condition during parameterization; thus the geomanlyze function is no longer necessary. Parameterization can be performed both with the built-in parametric solver and by wrapping a for-loop around the solver call.

# Backward Compatibility

#### GEOMETRY

The functionality corresponding to the following geometry functions from version 3.5a is not available in version 4.0a. Most of this functionality will be available in version 4.1.

- flim2curve, flcontour2mesh, and flmesh2spline
- geomspline, geomsurf

- loft
- helix
- arc
- geom0, geom1, geom2, and geom3
- geomedit
- geomfile
- tangent (scheduled for 4.0a)
- gencyl
- The paircand property of geomgroup

## MESH

The functionality corresponding to the following mesh functions from version 3.5a is not available in version 4.0a. Most of this functionality will be available in version 4.1.

- mesh2geom
- meshembed
- meshextrude and meshrevolve (essentially replaced by generalized sweep functionality)
- The hmesh and mesh properties of meshinit

# COMSOL API

See the section "The COMSOL API" on page 30 regarding changes in the COMSOL API.

# The COMSOL API

The following changes were made to the COMSOL API between version 4.0 and 4.0a:

- The load face parameter (Fph) of the *Phase* feature in AcousticStructure, TransientAcousticStructure, ThermallyInducedStresses, SolidMechanics, JouleHeatingThermalExpansion, Poroelasticity, and FluidStructureInteraction has changed interpretation from degrees to radians.
- physics.field() of Beam and Truss are not backward compatible with 4.0. Scalar fields are now vector fields.
- The variables for strain and stress in the Shell interface have been renamed. Variable names that began with lowercase s now begin with uppercase S. For variables names that ended in lowercase l (L), the letter was moved to the third position, e.g., emXX1 is now em1XX.
- Force loads on solids and trusses have been moved from material to spatial frame. This implies that index notation of some variables have changed from uppercase XYZ to lowercase xyz.
- The acoustics interfaces (PressureAcoustics, TransientPressureAcoustics, AcousticStructure, and TransientAcousticStructure) have been moved from material to spatial frame. This implies that index notation of vector variables have change from uppercase XYZ to lowercase xyz.

# New Terminology

The following tables include new terminology and names in version 4.0a and their corresponding equivalents in version 3.5a:

# GENERAL TERMINOLOGY

NAME IN 4.0	NAME IN 3.5A	COMMENTS
Parameters	Constants	Parameters in 4.0 have a broader scope, including the geometry. Also, predefined <i>physical constants</i> are new in 4.0.
Variables	Expressions, Expression variables	Variables appear in two locations depending on their scope: under Global Definitions with a global scope or under Definitions in each model. In the latter case, scope can be set to the entire model or to selected domains, boundaries, edges, or points.
Physics interface	Application mode	
Coupling operators	Coupling variables	You find the coupling operators under Model Couplings in the Definitions branches. A coupling operator, as opposed to a coupling variable, can be reused with different arguments. For example, the same coupling operator can be used to integrate different quantities over a boundary.
Hide	Suppress	For hiding part of the geometry in the Graphics window.
Study type	Analysis type	The study type sets up a study step, which controls the generation of a solver sequence for performing a certain type of study.
Results branch	Postprocessing menu	The Results branch contains the data sets for evaluation and visualizations of results as well as derived values, plot groups for various plots, tables for numerical results, and reports such as animations, data files, and images.
Convert to	Coerce to	For converting geometry objects from one type to another (for example, from a solid to a curve).
Domain	Subdomain	A solid geometry consists of one or several domains.

NAME IN 4.0	NAME IN 3.5A	COMMENTS
Bidirectional, symmetric constraint	Ideal constraint	In 4.0 available as a weak constraint and as a strong (pointwise) constraint.
Unidirectional constraint	Non-ideal constraint	In 4.0 available as a weak constraint and as a strong (pointwise) constraint.

# PHYSICS INTERFACES WITH NEW NAMES

NAME IN 4.0	NAMES IN 3.5A	COMMENTS
Transport of Diluted Species	Convection and Diffusion; Diffusion; Electrokinetic Flow; and Nernst-Planck without Electroneutrality	The Transport of Diluted Species interface includes all transport mechanism for mass transport of diluted species. The functionality for migration through electrophoresis and electroosmosis is only available in the Chemical Engineering Module and MEMS Module.
Transport of Concentrated Species	Maxwell-Stefan Diffusion and Convection	The Transport of Concentrated Species interface also includes two other diffusion models for mass transport of concentrated species: the mixture-averaged diffusion model and a diffusion model based on Fick's law.
Laminar Flow	Incompressible Navier-Stokes; non-Newtonian Flow; General Laminar Flow; and Stokes Flow	The Laminar Flow interface includes all variants of laminar flow. Some of the functionality is only available in the Chemical Engineering Module, Earth Science Module, Heat Transfer Module, and MEMS Module.
Electric Currents	Conductive Media DC; Quasi-Statics, Electric	The Electric Currents interface solves for the electric potential in applications where electric currents flow in a conductive media.
Heat Transfer in Solids	Conduction; General Heat Transfer	The Heat Transfer in Solids interface provides default settings for conductive heat transfer in solids. But you can easily switch from heat transfer in solids to heat transfer in fluids as well as add and combine different heat transfer mechanism within the same Heat Transfer interface.

NAME IN 4.0	NAMES IN 3.5A	COMMENTS
Heat Transfer in Fluids	Convection and Conduction; General Heat Transfer	The Heat Transfer in Fluids interface provides default settings for convective and conductive heat transfer in fluids. But you can easily switch from heat transfer in fluids to heat transfer in solids as well as add and combine different heat transfer mechanism within the same Heat Transfer interface.
Solid Mechanics	Solid, Stress-Strain; Axial Symmetry Stress-Strain; Plane Stress; and Plane Strain	In 2D models you can switch between plane stress and plane strain without adding a new physics interface.
Deformed Geometry	Parameterized Geometry	The Deformed Geometry interface is available for all geometries, not just 2D. In 4.0 it is also possible to study fully parameterized geometries using parametric sweeps.

# MATERIAL LIBRARIES

NAME IN 4.0	NAMES IN 3.5A	COMMENTS
Built-in	Basic Material Properties	Included in COMSOL Multiphysics.
MEMS	MEMS Material Properties	Included with the MEMS Module, Acoustics Module, and Structural Mechanics Module.
Piezoelectric	Piezoelectric Material Properties	Included with the MEMS Module, Acoustics Module, and Structural Mechanics Module.
AC/DC	Electric (AC/DC) Material Properties	Included with the AC/DC Module. The Samarium Cobalt material is no longer included.
Convective Cooling boundary condition	Heat Transfer Coefficients	In 4.0 the Convective Cooling boundary condition replaces the library of heat transfer coefficients. The Settings window for the Convective Cooling node contains predefined heat transfer coefficients for natural and forced convection (both internal and external). Included with the Heat Transfer Module.
Liquids and Gases	Liquids and Gases	Included with the Chemical Engineering Module, Acoustics Module, Earth Science Module, Heat Transfer Module, and MEMS Module.
Material Library	Material Library	The COMSOL Material Library add-on is unchanged.