COMSOL MULTIPHYSICS

CHEMICAL ENGINEERING MODULE

REFERENCE GUIDE

VERSION 3.4

COMSOL

How to contact COMSOL:

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

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

Finland
COMSOL OY
Arabianranta 6
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
FEMLAB GmbH
Berliner Str. 4
D-37073 Göttingen
Phone: +49-551-99721-0
Fax: +49-551-99721-29
info@femlab.de
www.femlab.de

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
FEMLAB GmbH
Technoparkstrasse 1
CH-8005 Zürich
Phone: +41 (0)44 445 2140
Fax: +41 (0)44 445 2141
info@femlab.ch
www.femlab.ch

United Kingdom
COMSOL Ltd.
UH Innovation Centre
College Lane
Hatfield
Hertfordshire AL10 9AB
Phone:+44-(0)-1707 284747
Fax: +44-(0)-1707 284746
info.uk@comsol.com
www.uk.comsol.com

United States
COMSOL, Inc.
1 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

Chemical Engineering Module Reference Guide

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Introduction

The Chemical Engineering Module 3.4 is an optional package that extends the COMSOL Multiphysics® modeling environment with customized user interfaces and functionality optimized for the analysis of with customized user interfaces and functionality optimized for the analysis of transport phenomena coupled to chemical reactions. Like all modules in the COMSOL family, it provides a library of prewritten ready-to-run models that make it quicker and easier to analyze discipline-specific problems.

The documentation set for the Chemical Engineering Module consists of two printed books, the *Chemical Engineering Module User's Guide* and the *Chemical Engineering Module Model Library*, and this *Chemical Engineering Module Reference Guide*, which is available in PDF and HTML versions from the COMSOL Help Desk. This book contains reference information such as application mode implementation details.

Typographical Conventions

All COMSOL manuals use a set of consistent typographical conventions that should make it easy for you to follow the discussion, realize what you can expect to

see on the screen, and know which data you must enter into various data-entry fields. In particular, you should be aware of these conventions:

- A **boldface** font of the shown size and style indicates that the given word(s) appear exactly that way on the COMSOL graphical user interface (for toolbar buttons in the corresponding tooltip). For instance, we often refer to the **Model Navigator**, which is the window that appears when you start a new modeling session in COMSOL; the corresponding window on the screen has the title **Model Navigator**. As another example, the instructions might say to click the **Multiphysics** button, and the boldface font indicates that you can expect to see a button with that exact label on the COMSOL user interface.
- The names of other items on the graphical user interface that do not have direct labels contain a leading uppercase letter. For instance, we often refer to the Draw toolbar; this vertical bar containing many icons appears on the left side of the user interface during geometry modeling. However, nowhere on the screen will you see the term "Draw" referring to this toolbar (if it were on the screen, we would print it in this manual as the **Draw** menu).
- The symbol **>** indicates a menu item or an item in a folder in the **Model Navigator**. For example, **Physics>Equation System>Subdomain Settings** is equivalent to: On the **Physics** menu, point to **Equation System** and then click **Subdomain Settings**. **COMSOL Multiphysics>Heat Transfer>Conduction** means: Open the **COMSOL Multiphysics** folder, open the **Heat Transfer** folder, and select **Conduction**.
- A `Code` (monospace) font indicates keyboard entries in the user interface. You might see an instruction such as "Type `1.25` in the **Current density** edit field." The monospace font also indicates COMSOL Script codes.
- An *italic* font indicates the introduction of important terminology. Expect to find an explanation in the same paragraph or in the Glossary. The names of books in the COMSOL documentation set also appear using an italic font.

2

Application Mode Implementations

The Chemical Engineering Module is built completely on top of COMSOL Multiphysics. It is divided into the three main branches of transport phenomena: momentum transport, energy transport, and mass transport. Each of these transport mechanisms has a number of associated application modes, based on the set of equations that are best suited for a certain phenomenon or application. All application modes are based on the PDE and weak modes defined in COMSOL Multiphysics.

The PDEs, boundary conditions, and theoretical background for each application mode are described in the chapters "Momentum Transport," "Energy Transport," "Mass Transport," and "Predefined Multiphysics Couplings" of the *Chemical Engineering Module User's Guide*.

This reference guide is a complement to the *Chemical Engineering Module User's Guide*. In the first section, "Application Mode Equations," you find a brief description of the PDE general form that all application modes are based on. There are also guidelines demonstrating how you can inspect the implementation of the equations, boundary conditions, and variables for an application mode in the graphical user interface.

The section “Application Mode Variables” lists the name and definitions of predefined application mode variables, which you can use in expressions and for postprocessing.

In the section “Log-Formulation of the Turbulence Equations” you find the logarithmic formulation of the turbulence equations that the turbulence application modes use.

The fourth section, “Special Element Types For Fluid Flow,” gives an overview of the available predefined element types available for the momentum transport application modes.

Application Mode Equations

The theoretical background, the subdomain equations and the boundary conditions for each application mode are presented in the *Chemical Engineering Module User's Guide*. This chapter describes how you can study how the equations are implemented in COMSOL Multiphysics using the graphical user interface.

All subdomain equations for the application modes in the Chemical Engineering Module are based on the following general form:

$$d_a\frac{\partial u}{\partial t} + \nabla \cdot (\Gamma) = F \tag{2-1}$$

To see how the equations for the application mode you are using are implemented in COMSOL Multiphysics, select **Equation System>Subdomain Settings** from the **Physics** menu. By selecting the $\mathbf{d_a}$, γ, and **f** page, you can inspect how the application mode defines d_a, Γ, and F, respectively. On the **Variables** page you find the subdomain variables defined by the application mode. On the **Weak** page you can see if the application mode adds any contributions to the weak form of the equations. The weak form of Equation 2-1 is

$$\int_\Omega u_{\text{test}} F d\Omega - \int_\Omega u_{\text{test}}\left(d_a\frac{\partial u}{\partial t} + \nabla \cdot (\Gamma)\right)d\Omega = 0$$

or, using integration by parts,

$$\int_\Omega u_{\text{test}} F d\Omega - \int_\Omega u_{\text{test}}\left(d_a\frac{\partial u}{\partial t}\right)d\Omega + \int_\Omega \nabla u_{\text{test}} \cdot \Gamma d\Omega - \int_{\partial\Omega} u_{\text{test}}(\Gamma \cdot \mathbf{n}) d\partial\Omega = 0$$

The boundary conditions are specified on the form

$$R = 0$$

$$-\mathbf{n} \cdot \Gamma = G - \left(\frac{\partial R}{\partial u}\right)^T \mu$$

where $\mathbf{n}$ is the boundary outward unit normal vector. By choosing **Equation System>Boundary Settings** from the **Physics** menu, you can view how R and G are defined from the expressions on the **r** and **g** pages. Additional constraints can be found in the **constr** edit field on the **Weak** page. On the **Variables** page you find a list of all application mode variables defined on the boundaries.

Note that you can modify the subdomain equations, boundary conditions, and definition of the application mode variables by editing the expressions in the different **Equation System** dialog boxes.

Application Mode Variables

The application modes in the Chemical Engineering Module define a large set of variables. This chapter contains lists of the the variables that each application mode defines. Other information, like the theoretical background for the application modes, can be found in the *Chemical Engineering Module User's Guide*.

Most application modes define variables of three different types. The *dependent variables* are the unknowns solved for. They are represented using shape functions, and are essential to any problem, that is, they cannot be replaced by numerical values or expressions in terms of other variables. You can specify names for the dependent variables when you select an application mode in the Model Navigator. Below, the default names are listed for each application mode.

The *application scalar variables* are normally numerical values, for example universal constants, model parameters and user-controlled constants such as the frequency of a harmonic oscillation. In rare cases, they can also be globally defined expressions in terms of other application mode variables. In the following sections, any application scalar variables are presented in a table together with their default value, unit and description.

Remaining variables defined by the application mode, collectively referred to as *application mode variables*, are expressions defined in terms of other variables and constants on domains of a specific dimension. Further, the definition can vary from domain to domain, depending on the currently applied physics settings. The application mode variable tables in the following sections are organized as follows:

- The **Name** column lists the names of the variables that you can use in expressions in the equations or for postprocessing. Note that some variables represent vector- or tensor-valued expressions. In that case, there is one variable for each component, using the independent variable names as index. For example, if the table writes the variable name as `T_`x_i, the actual variables are typically called `T_x` and `T_y` in 2D Cartesian coordinates and `T_r`, `T_z` in axisymmetric geometries.

Note: All variables defined by the application mode, except the dependent variables, get an underscore plus the application mode name appended to them. For example, the default application mode name for the Incompressible Navier-Stokes application mode is `chns`, hence, the density variable name is `rho_chns`.

- The **Type** column indicates if the variable is defined on subdomains (S), boundaries (B), edges (E), or points (P). The column indicates the levels where the variable is explicitly declared. Variables that are not explicit on domains of a given dimension can nevertheless be evaluated if they are declared in an adjacent domain of higher dimension. When there is more than one adjacent domain, an average value is computed. For example, all subdomain variables can also be evaluated on boundaries, but on interior boundaries take on the mean of the values in the two adjacent subdomains.

  The **Type** column can also show a (V) or (T) to indicate that the variable is a component of a vector or tensor. Vector variables are included in the lists of predefined expressions for plot types such as Arrow, Deform and Streamline.
- The **Description** column gives a description of the variables.
- The **Expression** column gives the expression of the variables in terms of other variables or physical quantities, or a reference to an explanation elsewhere.

The application mode variables listed in the following sections are all available both for postprocessing and when formulating the equations. Note that you can also find the definitions of these variables directly in the graphical user interface of COMSOL Multiphysics. From the **Physics** menu, choose **Scalar Variables** to inspect the application scalar variables, or select one of the items in the **Equation System** submenu to open the **Equation System** dialog box for the corresponding dimension. On the **Variables** page, you will find the application mode variable names and their definitions (which you can also change, if you like).

Note that the actual variable names in your model may depend on the spatial coordinate names, as well as on the order in which application modes are added to a Multiphysics model. The names and definitions may also be affected by application mode property settings and by the physics settings for the particular subdomain or boundary. Therefore, it is good practice to always check the variable names for your particular model in the GUI, before using them in equations.

Momentum Transport Application Modes

This chapter contains tables of the application mode names, the dependent variables, the scalar variables and the application mode variables for all the Momentum Transport application modes.

INCOMPRESSIBLE NAVIER-STOKES

APPLICATION MODE NAME
chns

TABLE 2-1: DEPENDENT VARIABLES, INCOMPRESSIBLE NAVIER-STOKES

NAME	DESCRIPTION
u, v, w	Velocity in the x_1, x_2, and x_3 directions
p	Pressure

TABLE 2-2: APPLICATION MODE VARIABLES, INCOMPRESSIBLE NAVIER-STOKES

NAME	TYPE	DESCRIPTION	EXPRESSION
rho	S	Density	ρ
eta	S	Dynamic viscosity	η
F	S	Volume force	$\mathbf{F}$
U	S	Velocity field	$\lvert\mathbf{u}\rvert$
V	S	Vorticity	$\nabla \times \mathbf{u}$
K	B	Viscous force per unit area	$[\eta(\nabla\mathbf{u} + (\nabla\mathbf{u})^T)] \cdot \mathbf{n}$
T	B	Total force per unit area	$[\eta(\nabla\mathbf{u} + (\nabla\mathbf{u})^T) - p\mathbf{I}] \cdot \mathbf{n}$
cellRe	S	Cell Reynolds number	$\frac{\rho\lvert\mathbf{u}\rvert h}{\eta}$
res	S	Equation residual	$\rho\mathbf{u}_t + \rho(\mathbf{u}\cdot\nabla)\mathbf{u} + \nabla p - \mathbf{F} - \nabla\cdot[\eta(\nabla\mathbf{u} + (\nabla\mathbf{u})^T)]$
res_sc	S	Shock capturing residual	$\rho\mathbf{u}_t + \rho(\mathbf{u}\cdot\nabla)\mathbf{u} + \nabla p - \mathbf{F}$
beta	S	Convective term	$\rho\mathbf{u}$
da	S	Total time-scale factor	ρ
divU	S	Divergence of velocity field	$\nabla\cdot\mathbf{u}$
taum	S	GLS time scale	$\min\left(\frac{\Delta t}{\rho}, \frac{0.5h}{\max\left(\rho\lvert\mathbf{u}\rvert, \frac{6\eta}{h}\right)}\right)$
tauc	S	GLS time scale	$0.5\lvert\mathbf{u}\rvert h\min\left(1, \frac{\rho\lvert\mathbf{u}\rvert h}{\eta}\right)$

TABLE 2-2: APPLICATION MODE VARIABLES, INCOMPRESSIBLE NAVIER-STOKES

NAME	TYPE	DESCRIPTION	EXPRESSION
Dm	S	Mean diffusion coefficient	η
u0, v0, w0	B	Velocity (Velocity BC)	$\mathbf{u}_0$
p0	B	Pressure (Pressure BC)	p_0
f0	B	Normal stress (Normal stress BC)	f_0
Fbnd	B	Stress (General stress BC)	$\mathbf{F}$
U0in	B	Normal inflow velocity (Velocity BC)	U_0
U0out	B	Normal outflow velocity (Velocity BC)	U_0
uvw	B	Velocity of tangentially moving wall (Sliding wall BC, 2D)	$\mathbf{u}_\mathrm{w}$
uw, vw, ww	B	Velocity of tangentially moving wall (Sliding wall BC, 3D)	$\mathbf{u}_\mathrm{w}$
uwall	B	Velocity of moving wall (Moving/Leaking wall BC)	$\mathbf{u}_\mathrm{w}$
U0	B	Average velocity (laminar inflow/outflow BC)	U_0
V0	B	Volume per time unit (laminar inflow/outflow BC 3D)	V_0
Lentr	B	Entrance length (laminar inflow BC)	L_entr
Lexit	B	Exit length (laminar outflow BC)	L_exit
p0_entr	B	Entrance pressure (laminar inflow BC)	$p_{0,\mathrm{entr}}$
p0_exit	B	Exit pressure (laminar outflow BC)	$p_{0,\mathrm{exit}}$

SWIRL FLOW

APPLICATION MODE NAME
chns

TABLE 2-3: DEPENDENT VARIABLES, SWIRL FLOW

NAME	DESCRIPTION
u, v, w	Velocity in the r, z, and φ directions
p	Pressure

The application mode variables are identical to those of the Incompressible Navier-Stokes, see Table 2-2.

NON-NEWTONIAN FLOW

APPLICATION MODE NAME
chns

DEPENDENT VARIABLES, NON-NEWTONIAN FLOW

NAME	DESCRIPTION
u, v, w	Velocity in the x_1, x_2, and x_3 directions
p	Pressure

In addition to the application mode variables available for the Incompressible Navier-Stokes application mode (Table 2-2), the following variables are also available for Non-Newtonian Flow.

TABLE 2-4: APPLICATION MODE VARIABLES, NON-NEWTONIAN FLOW

NAME	TYPE	DESCRIPTION	EXPRESSION
m	S	Power Law model; power law parameter	m
n	S	Power Law model; shear thinning index	n
eta_inf	S	Carreau model; infinite shear rate viscosity	η_∞
eta_0	S	Carreau model; zero shear rate viscosity	η_0
lambda	S	Carreau model; Carreau model parameter	λ
sr	S	Shear rate	$\dot{\gamma}$
eta	S	Dynamic viscosity	η

The non-Newtonian viscosity, η, is defined as:

TABLE 2-5: NON-NEWTONIAN FLOW—EQUATIONS FOR VISCOSITY

VISCOSITY MODEL	EXPRESSION
Power Law	$\eta = m\dot{\gamma}^{n-1}$
Carreau	$\eta = \eta_\infty + (\eta_0 - \eta_\infty)[1 + (\lambda\dot{\gamma})^2]^{\frac{(n-1)}{2}}$

and the shear rate, $\dot{\gamma}$, is defined as:

TABLE 2-6: NON-NEWTONIAN FLOW—EQUATIONS FOR SHEAR RATE

$\dot{\gamma}$ 2D	$\sqrt{\frac{1}{2}\left(4\frac{\partial u}{\partial x}^2 + 2\left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right)^2 + 4\frac{\partial v}{\partial y}^2\right)}$
$\dot{\gamma}$ Axi 2D	$\sqrt{\frac{1}{2}\left(4\frac{\partial u}{\partial r}^2 + 2\left(\frac{\partial u}{\partial z} + \frac{\partial v}{\partial r}\right)^2 + 4\frac{\partial v}{\partial z}^2 + 4\left(\frac{u}{r}\right)^2\right)}$
$\dot{\gamma}$ 3D	$\sqrt{\frac{1}{2}\left(4\frac{\partial u}{\partial x}^2 + 4\frac{\partial v}{\partial y}^2 + 4\frac{\partial w}{\partial z}^2 + 2\left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right)^2 + 2\left(\frac{\partial v}{\partial z} + \frac{\partial w}{\partial y}\right)^2 + 2\left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x}\right)^2\right)}$

TURBULENT FLOW, K-ε TURBULENCE MODEL

APPLICATION MODE NAME
chns

TABLE 2-7: DEPENDENT VARIABLES, K-ε TURBULENCE MODEL

NAME	DESCRIPTION
u, v, w	Velocity in the x_1, x_2, and x_3 directions
p	Pressure
logk	Logarithm of turbulent kinetic energy
logd	Logarithm of turbulent dissipation rate

Table 2-8 shows the different scalar variables used in the k-ε Turbulence Model application mode:

TABLE 2-8: SCALAR VARIABLES, K-ε TURBULENCE MODEL

NAME	DESCRIPTION	EXPRESSION
Cmu	Turbulence modeling constant (= 0.09)	C_μ
Cd1	Turbulence modeling constant (= 1.44)	$C_{d1} = C_{\varepsilon 1}$

TABLE 2-8: SCALAR VARIABLES, K-ε TURBULENCE MODEL

NAME	DESCRIPTION	EXPRESSION
Cd2	Turbulence modeling constant (= 1.92)	$C_{d2} = C_{\varepsilon 2}$
sigmak	Turbulence modeling constant (= 1.0)	σ_k
sigmad	Turbulence modeling constant (= 1.3)	σ_ε
kappa	von Kármán constant (=0.42)	κ
Cplus	Logarithmic wall function constant (= 5.5)	C^+

In addition to the application mode variables available for the Incompressible Navier-Stokes application mode, the following variables are available.

TABLE 2-9: APPLICATION MODE VARIABLES, K-ε TURBULENCE MODEL

NAME	TYPE	DESCRIPTION	EXPRESSION
k0	S	Turbulent kinetic energy	$k = e^{\log k}$
d0	S	Turbulent dissipation rate	$\varepsilon = e^{\log d}$
etaT	S	Turbulent viscosity	$\rho C_\mu \frac{k^2}{\varepsilon}$

TURBULENT FLOW, K-ω TURBULENCE MODEL

APPLICATION MODE NAME
chns

TABLE 2-10: DEPENDENT VARIABLES, K-ω TURBULENCE MODEL

NAME	DESCRIPTION
u, v, w	Velocity in the x_1, x_2, and x_3 directions
p	Pressure
logk	Logarithm of turbulent kinetic energy
logw	Log of specific turbulent dissipation rate

Table 2-11 summarizes the different scalar variables used in the k-ω Turbulence Model application mode:

TABLE 2-11: SCALAR VARIABLES, K-ω TURBULENCE MODEL

NAME	DESCRIPTION	EXPRESSION
Cmu	Turbulence modeling constant (= 0.09)	C_μ
alpha	Turbulence modeling constant (= 13/25)	α
beta0	Turbulence modeling constant (= 9/125)	β_0
beta0k	Turbulence modeling constant (= 0.09)	$\beta_{0,k}$
sigmaw	Turbulence modeling constant (= 0.5)	σ_ω
kappa	von Kármán constant (=0.42)	κ
Cplus	Logarithmic wall function constant (= 5.5)	C^+

In addition to the application mode variables available for the Incompressible Navier-Stokes application mode, the following variables are available.

TABLE 2-12: APPLICATION MODE VARIABLES, K-ω TURBULENCE MODEL

LABEL	TYPE	DESCRIPTION	EXPRESSION
k0	S	Turbulent kinetic energy	$k = e^{\log k}$
omega0	S	Specific turbulent dissipation rate	$\omega = e^{\log w}$
etaT	S	Turbulent viscosity	$\rho e^{\log k - \log w}$

DARCY'S LAW

APPLICATION MODE NAME
chdl

TABLE 2-13: DEPENDENT VARIABLES, DARCY'S LAW

NAME	DESCRIPTION
p	Pressure

The following application mode variables are available:

TABLE 2-14: APPLICATION MODE VARIABLES, DARCY'S LAW

NAME	TYPE	DESCRIPTION	EXPRESSION
gradP	S	Pressure gradient	$\|\nabla p\|$
u, v, w	S	Velocity components	$-\frac{\kappa}{\eta}\nabla p$
U	S	Velocity field	$\frac{\kappa}{\eta}\|\nabla p\|$
u0	B	Inward velocity	u_0
Dts	S	Time-scaling coefficient	δ_{ts}
k	S	Permeability	κ
rho	S	Density	ρ
eta	S	Viscosity	η
F	S	Source term	F
epsilon	S	Volume fraction	ε

THE BRINKMAN EQUATIONS

APPLICATION MODE NAME
chns

TABLE 2-15: DEPENDENT VARIABLES, BRINKMAN EQUATIONS

NAME	DESCRIPTION
u, v, w	Velocity in the x_1, x_2, and x_3 directions
p	Pressure

The application mode variables are identical to those for the Incompressible Navier-Stokes application mode, given in Table 2-2.

THE LEVEL SET METHOD

APPLICATION MODE NAME
mmls

TABLE 2-16: DEPENDENT VARIABLES, LEVEL SET

NAME	DESCRIPTION
phi	Level set variable

TABLE 2-17: APPLICATION MODE VARIABLES, LEVEL SET

NAME	TYPE	DESCRIPTION	EXPRESSION
gamma	S	Reinitialization parameter	γ
epsilon	S	Parameter controlling interface thickness	ε
u	S	Velocity	$\mathbf{u}$
gradphi	S	Gradient of phi	$\nabla\phi$
norm	S	Interface normal	$\mathbf{n}_{\text{interface}} = \frac{\nabla\phi}{\lvert\nabla\phi\rvert}$
kappa	S	Mean curvature	$(-\nabla \cdot \mathbf{n}_{\text{interface}})(\phi > 0.1)(\phi < 0.9)$
hmaxi	S	Maximum mesh size in subdomain i	
hmax	S	Maximum mesh size in each subdomain	

THE LEVEL SET METHOD FOR TWO-PHASE FLOW

APPLICATION MODE NAME
chns

TABLE 2-18: DEPENDENT VARIABLES, LEVEL SET TWO-PHASE FLOW

NAME	DESCRIPTION	APPLICATION MODE PROPERTY
u, v, w	Velocity in the x_1, x_2, and x_3 directions	
p	Pressure	
phi	Level set variable	
logk	Logarithm of turbulent kinetic energy	k-eps
logd	Logarithm of turbulent dissipation rate	k-eps

The Level Set Two Phase Flow application mode contains all the variables for Incompressible Navier-Stokes (Table 2-2) and Level Set (Table 2-17). For Level Set Two Phase Flow, *k*-ε Turbulence Model, the variables in Table 2-9 are also available. In addition to that, the following application mode variable is available:

TABLE 2-19: APPLICATION MODE VARIABLE, LEVEL SET TWO PHASE FLOW

NAME	TYPE	DESCRIPTION	EXPRESSION
delta	S	Dirac delta function	$6\|\nabla\phi\|\|\phi(1-\phi)\|$
Vf1	S	Volume fraction of fluid 1	$1-\phi$
Vf2	S	Volume fraction of fluid 2	ϕ

BUBBLY FLOW MODEL

APPLICATION MODE NAME
chbf

TABLE 2-20: DEPENDENT VARIABLES, BUBBLY FLOW

NAME	DESCRIPTION	APPLICATION MODE PROPERTY
ul, vl, wl	Liquid velocity	
p	Pressure	
rhogeff	Effective gas density	
logk	Logarithm of turbulent kinetic energy	k-eps
logd	Logarithm of turbulent dissipation rate	k-eps
nbub	Bubble number density	Interfacial area/ volume

TABLE 2-21: SCALAR VARIABLES, BUBBLY FLOW

NAME	DESCRIPTION	EXPRESSION
Cmu	Turbulence modeling constant (= 0.09)	C_μ
Cd1	Turbulence modeling constant (= 1.44)	$C_{d1} = C_{\varepsilon 1}$
Cd2	Turbulence modeling constant (= 1.92)	$C_{d2} = C_{\varepsilon 2}$
sigmak	Turbulence modeling constant (= 1.0)	σ_k
sigmad	Turbulence modeling constant (= 1.3)	σ_ε
kappa	von Kármán constant (= 0.42)	κ
Cplus	Logarithmic wall function constant (= 5.5)	C^+
Ck	Bubble-induced turbulence modeling constant (= 1.0)	C_k
Ce	Bubble-induced turbulence modeling constant (=1.0)	C_ε
R	Universal gas constant (= 8.315 J/(mol·K))	R
pref	Reference pressure(=10^5 Pa)	p_{ref}

TABLE 2-22: APPLICATION MODE VARIABLES, BUBBLY FLOW

NAME	TYPE	DESCRIPTION	EXPRESSION
rhol	S	Density of pure liquid	ρ_l
etal	S	Dynamic viscosity of pure liquid	η_l
T	S	Temperature	T

TABLE 2-22: APPLICATION MODE VARIABLES, BUBBLY FLOW

NAME	TYPE	DESCRIPTION	EXPRESSION
M	S	Molecular weight of gas	M
grav	S	Gravity vector	$\mathbf{g}$
F	S	Volume force	$\mathbf{F}$
diam	S	Bubble diameter	d_b
sigma	S	Surface tension coefficient	σ
Cdud	S	User-defined drag coefficient	C_d
henry	S	Henry's constant	H
kmasstrans	S	Mass transfer coefficient	k
c	S	Concentration of species dissolved in liquid	c
masstransud	S	User-defined mass transfer rate	m_gl
uslip, vslip, wslip	S	Slip velocity, small bubbles	$\mathbf{u}_\mathrm{slip} = -\frac{\nabla p\, d_\mathrm{b}^2}{12\eta_\mathrm{l}}$
uslip, vslip, wslip	S	Slip velocity, large bubble or user-defined drag coefficient	$\mathbf{u}_\mathrm{slip} = -\sqrt{\frac{4d_\mathrm{b}}{3C_\mathrm{d}\rho_\mathrm{l}\lvert\nabla p\rvert}}\nabla p$
Cdrag	S	Drag coefficient, large bubbles	$C_\mathrm{d} = \frac{0.622}{\frac{1}{\mathrm{E\ddot{o}}} + 0.235}$
Cdrag	S	Drag coefficient, small bubbles	$C_\mathrm{d} = \frac{16}{\mathrm{Re}_\mathrm{b}}$
Reb	S	Bubble Reynolds number	$\frac{d_\mathrm{b}\rho_\mathrm{l}\lvert\mathbf{u}_\mathrm{slip}\rvert}{\eta_\mathrm{l}}$
Eotvos	S	Eotvos number	$\frac{g\rho_\mathrm{l}d_\mathrm{b}^2}{\sigma}$
rhog	S	Gas density	$\frac{(p+p_\mathrm{ref})M}{RT}$

TABLE 2-22: APPLICATION MODE VARIABLES, BUBBLY FLOW

NAME	TYPE	DESCRIPTION	EXPRESSION
phig	S	Volume fraction of gas	$\frac{\rho_{geff}}{\rho_g}$
phil	S	Volume fraction of liquid	$1-\phi_g$
masstrans	S	Mass transfer rate, two film theory	$\mathrm{Ek}\left(\frac{p+p_{ref}}{H}-c\right)\mathrm{Ma}$
a	S	Interfacial area per unit volume	$(4n_{bub}\pi)^{1/3}(3\phi_g)^{2/3}$
ug, vg, wg	S	Gas phase velocity	$\mathbf{u}_l+\mathbf{u}_{slip}+\mathbf{u}_{drift}$
udrift, vdrift, wdrift	S	Bubble drift velocity (k-ε Turbulence model)	$-\frac{\eta_T}{\rho_l}\frac{\nabla\phi_g}{\phi_g}$
etaT	S	Turbulent viscosity (k-ε Turbulence model)	$\rho_l C_\mu \frac{k^2}{\varepsilon}$

THE MIXTURE MODEL

APPLICATION MODE NAME
chmm

TABLE 2-23: DEPENDENT VARIABLES, MIXTURE MODEL

NAME	DESCRIPTION	APPLICATION MODE PROPERTY
u, v, w	Mixture velocity	
p	Pressure	
phid	Volume fraction of dispersed phase	
logk	Logarithm of turbulent kinetic energy	k-eps
logd	Logarithm of turbulent dissipation rate	k-eps
slipvel	Squared slip velocity	Schiller-Naumann
nd	Number density	Interfacial area/volume

TABLE 2-24: SCALAR VARIABLES, MIXTURE MODEL

NAME	DESCRIPTION	EXPRESSION
Cmu	Turbulence modeling constant (= 0.09)	C_{μ}
Cd1	Turbulence modeling constant (= 1.44)	$C_{d1} = C_{\varepsilon 1}$
Cd2	Turbulence modeling constant (= 1.92)	$C_{d2} = C_{\varepsilon 2}$
sigmak	Turbulence modeling constant (= 1.0)	σ_k
sigmad	Turbulence modeling constant (= 1.3)	σ_{ε}
kappa	von Kármán constant (= 0.42)	κ
sigmaT	Turbulent particle Schmidt number (= 0.35)	σ_T
Cplus	Logarithmic wall function constant (= 5.5)	C^+

TABLE 2-25: APPLICATION MODE VARIABLES, MIXTURE MODEL

NAME	TYPE	DESCRIPTION	EXPRESSION
rhoc	S	Density of continuous phase	ρ_c
etac	S	Dynamic viscosity of continuous phase	η_c
rhod	S	Density of dispersed phase	ρ_d

TABLE 2-25: APPLICATION MODE VARIABLES, MIXTURE MODEL

NAME	TYPE	DESCRIPTION	EXPRESSION
etad	S	Dynamic viscosity of dispersed phase	η_{d}
diam	S	Diameter of dispersed phase particles	d_{d}
grav	S	Gravity vector	$\mathbf{g}$
F	S	Volume force	$\mathbf{F}$
phimax	S	Maximum packing concentration	$\phi_{\max}$
kmasstrans	S	Mass transfer coefficient	k
concd	S	Concentration, dispersed phase	c_{d}
concc	S	Concentration, continuous phase	c_{c}
M	S	Molecular weight	M
masstransud	S	Mass transfer from dispersed to continuous phase	m_{dc}
masstrans	S	Mass transfer, two-film theory	$k(c_{\mathrm{d}}-c_{\mathrm{c}})\mathrm{Ma}$
a	S	Interfacial area/volume	$a = (4n\pi)^{1/3}(3\phi_{\mathrm{d}})^{2/3}$
phic	S	Volume fraction of continuous phase	$\phi_{\mathrm{c}} = 1-\phi_{\mathrm{d}}$
rho	S	Mixture density	$\phi_{\mathrm{c}}\rho_{\mathrm{c}}+\phi_{\mathrm{d}}\rho_{\mathrm{d}}$
cd	S	Mass fraction of dispersed phase	$\frac{\phi_{\mathrm{d}}\rho_{\mathrm{d}}}{\rho}$
Rep	S	Particle Reynolds number, Schiller-Naumann	$\frac{d_{\mathrm{d}}\rho_{\mathrm{c}}}{\eta}\sqrt{\mathrm{slipvel}}$
Cdrag	S	Drag coefficient, Schiller-Naumann	$\max\left(\frac{24}{\mathrm{Re}_p}((1+0.15\mathrm{Re}_p^{0.687}),0.44)\right)$
ud, vd, wd	S	Dispersed phase velocity	$\mathbf{u}+(1-c_{\mathrm{d}})\mathbf{u}_{\mathrm{slip}}-D_{m\mathrm{d}}\frac{\nabla\phi_{\mathrm{d}}}{\phi_{\mathrm{d}}+\mathrm{eps}}$

TABLE 2-25: APPLICATION MODE VARIABLES, MIXTURE MODEL

NAME	TYPE	DESCRIPTION	EXPRESSION
uc, vc, wc	S	Continuous phase velocity	$\frac{\mathbf{u}-c_{\mathrm{d}}\mathbf{u}_{\mathrm{d}}}{1-c_{\mathrm{d}}}$
Dmd	S	Diffusion coefficient for dispersed phase due to turbulence	$\frac{\eta_T}{\rho\sigma_T}$
uslip, vslip, wslip	S	Slip velocity, Hadamard-Rybczynski, liquid droplets/bubbles	$-\frac{(\rho-\rho_{\mathrm{d}})d_{\mathrm{d}}^2}{18\rho\eta}\left(\frac{1+\frac{\eta_{\mathrm{c}}}{\eta_{\mathrm{d}}}}{1+\frac{2}{3}\frac{\eta_{\mathrm{c}}}{\eta_{\mathrm{d}}}}\right)\nabla p$
uslip, vslip, wslip	S	Slip velocity, Hadamard-Rybczynski, solid particles	$-\frac{(\rho-\rho_{\mathrm{d}})d_{\mathrm{d}}^2}{18\rho\eta}\nabla p$
uslip, vslip, wslip_	S	Slip velocity, Schiller-Naumann	$-\sqrt{\mathrm{slipvel}}\frac{(\rho-\rho_{\mathrm{d}})\nabla p}{\lvert(\rho-\rho_{\mathrm{d}})\rvert\lvert\nabla p\rvert}$
eta	S	Mixture viscosity, Krieger type model, solid particles	$\eta_{\mathrm{c}}\left(1-\frac{\phi_{\mathrm{d}}}{\phi_{\max}}\right)^{-2.5\phi_{\max}}$
eta	S	Mixture viscosity, Krieger type model, droplets/bubbles	$\eta_{\mathrm{c}}\left(1-\frac{\phi_{\mathrm{d}}}{\phi_{\max}}\right)^{-2.5\phi_{\max}\frac{\eta_d+0.4\eta_c}{\eta_d+\eta_c}}$
eta	S	Mixture viscosity, Volume averaged	$\eta = \phi_{\mathrm{d}}\eta_{\mathrm{d}}+(1-\phi_{\mathrm{d}})\eta_{\mathrm{c}}$

WEAKLY COMPRESSIBLE NAVIER-STOKES

APPLICATION MODE NAME
chns

TABLE 2-26: DEPENDENT VARIABLES, WEAKLY COMPRESSIBLE NAVIER-STOKES

NAME	DESCRIPTION
u, v, w	Velocity in the x_1, x_2, and x_3 directions
p	Pressure

The application mode variables are:

TABLE 2-27: APPLICATION MODE VARIABLES, WEAKLY COMPRESSIBLE NAVIER-STOKES

NAME	TYPE	DESCRIPTION	EXPRESSION
rho	S	Density	ρ
eta	S	Dynamic viscosity	η
kappadv	S	Dilatational viscosity	κ
F	S	Volume force	$\mathbf{F}$
U	S	Velocity field	$\|\mathbf{u}\|$
V	S	Vorticity	$\nabla \times \mathbf{u}$
K	B	Viscous force per area	$\left[\eta(\nabla\mathbf{u} + (\nabla\mathbf{u})^T) - \left(\frac{2\eta}{3} - \kappa\right)(\nabla \cdot \mathbf{u})\mathbf{I}\right] \cdot \mathbf{n}$
T	B	Total force per area	$\left[-p\mathbf{I} + \eta(\nabla\mathbf{u} + (\nabla\mathbf{u})^T) - \left(\frac{2\eta}{3} - \kappa\right)(\nabla \cdot \mathbf{u})\mathbf{I}\right] \cdot \mathbf{n}$
cellRe	S	Cell Reynolds number	$\frac{\rho\|\mathbf{u}\|h}{\eta}$
res	S	Equation residual	$\rho\mathbf{u}_t + \rho(\mathbf{u} \cdot \nabla)\mathbf{u} + \nabla p - \mathbf{F} - \nabla \cdot \left[\eta(\nabla\mathbf{u} + (\nabla\mathbf{u})^T) - \left(\frac{2\eta}{3} - \kappa\right)(\nabla \cdot \mathbf{u})\mathbf{I}\right]$
res_sc	S	Shock capturing residual	$\rho\mathbf{u}_t + \rho(\mathbf{u} \cdot \nabla)\mathbf{u} + \nabla p - \mathbf{F}$
beta	S	Convective field	$\rho\mathbf{u}$
Dm	S	Mean diffusion coefficient	η

TABLE 2-27: APPLICATION MODE VARIABLES, WEAKLY COMPRESSIBLE NAVIER-STOKES

NAME	TYPE	DESCRIPTION	EXPRESSION
da	S	Total time-scale factor	ρ
divU	S	Divergence of velocity field	$\nabla \cdot \mathbf{u}$
taum	S	GLS time scale	$\min\left(\frac{\Delta t}{\rho}, \frac{0.5h}{\max\left(\rho\lvert\mathbf{u}\rvert, \frac{6\eta}{h}\right)}\right)$
tauc	S	GLS time scale	$0.5\lvert\mathbf{u}\rvert h \min\left(1, \frac{\rho\lvert\mathbf{u}\rvert h}{\eta}\right)$

Energy Transport Application Modes

This chapter contains tables of the application mode names, the dependent variables, the scalar variables and the application mode variables for all the Energy Transport application modes.

CONVECTION AND CONDUCTION

APPLICATION MODE NAME
chcc

TABLE 2-28: DEPENDENT VARIABLES, CONVECTION AND CONDUCTION

NAME	DESCRIPTION
T	Temperature

The application mode variables are:

TABLE 2-29: APPLICATION MODE VARIABLES, CONVECTION AND CONDUCTION

NAME	TYPE	DESCRIPTION	EXPRESSION
grad_T	S	Temperature gradient	∇T
dflux	S (V)	Conductive flux	$-k\nabla T$
cflux	S (V)	Convective flux	$\rho C_p T\mathbf{u}$
tflux	S (V)	Total heat flux	$-k\nabla T + \rho C_p T\mathbf{u}$
ndflux	B	Normal conductive flux	$\mathbf{n} \cdot (-k\nabla T)$

TABLE 2-29: APPLICATION MODE VARIABLES, CONVECTION AND CONDUCTION

NAME	TYPE	DESCRIPTION	EXPRESSION
ncflux	B	Normal convective flux	$\rho C_p T \mathbf{n} \cdot \mathbf{u}$
ntflux	B	Normal total heat flux	$\mathbf{n} \cdot (-k\nabla T + \rho C_p T \mathbf{u})$
cellPe	S	Cell Peclet number	$\left\lvert \frac{\rho C_p \mathbf{u} h}{D_m} \right\rvert$
Dts	S	Time-scale factor	δ_{ts}
rho	S	Density	ρ
C	S	Heat capacity	C_p
k	S	Thermal conductivity	k
Q	S	Heat source	Q
u, v, w	S	Velocity	$\mathbf{u}$
Dm	S	Mean diffusion coefficient	$\frac{\sum_{i,j} k_{ij}\beta_i\beta_j}{\lvert\beta\rvert}$, $\beta = \rho C_p \mathbf{u}$
res	S	Equation residual	$\nabla \cdot (-k\nabla T + \rho C_p T \mathbf{u}) - Q$
res_sc	S	Shock-capturing residual	$\nabla \cdot (\rho C_p T \mathbf{u}) - Q$

CONDUCTION

APPLICATION MODE NAME
ht

TABLE 2-30: DEPENDENT VARIABLES, CONDUCTION

NAME	DESCRIPTION
T	Temperature

The application mode variables are:

TABLE 2-31: APPLICATION MODE VARIABLES, CONDUCTION

NAME	TYPE	DESCRIPTION	EXPRESSION
gradT	S	Temperature gradient	∇T
flux	S (V)	Heat flux	$-k\nabla T$
nflux	B	Normal heat flux	$\mathbf{n} \cdot (-k\nabla T)$

TABLE 2-31: APPLICATION MODE VARIABLES, CONDUCTION

NAME	TYPE	DESCRIPTION	EXPRESSION
Dts	S	Time-scaling coefficient	δ_{ts}
rho	S	Density	ρ
C	S	Heat capacity	C_p
k	S	Thermal conductivity	k
Q	S	Heat source	Q
htrans	S	Transversal convective heat transfer coefficient	h_{trans}
Text	S	Transversal external temperature	T_{ext}
Ctrans	S	User-defined constant	C_{trans}
Tambtrans	S	Transversal ambient temperature	T_{ambtrans}
T0	B	Prescribed temperature	T_0
h	B	Convective heat transfer coefficient	h
Tinf	B	Ambient bulk temperature	T_{inf}
Const	B	Radiation constant: product of emissivity and Stefan-Boltzmann constant	Const
Tamb	B	Temperature of the surrounding radiating environment	T_{amb}

Mass Transport Application Modes

This chapter contains tables of the application mode names, the dependent variables, the scalar variables and the application mode variables for all the Mass Transport application modes.

CONVECTION AND DIFFUSION

APPLICATION MODE NAME
chcd

TABLE 2-32: DEPENDENT VARIABLES, CONVECTION AND DIFFUSION

NAME	DESCRIPTION
c	Concentration

The application mode variables are:

TABLE 2-33: APPLICATION MODE VARIABLES, CONVECTION AND DIFFUSION

NAME	TYPE	DESCRIPTION	EXPRESSION
grad	S	Concentration gradient	∇c
dflux	S (V)	Diffusive flux	$-D\nabla c$
cflux	S (V)	Convective flux	$c\mathbf{u}$
tflux	S (V)	Total flux	$-D\nabla c + c\mathbf{u}$
ndflux	B	Normal diffusive flux	$\mathbf{n} \cdot (-D\nabla c)$
ncflux	B	Normal convective flux	$c\mathbf{n}\cdot\mathbf{u}$
ntflux	B	Normal total flux	$\mathbf{n} \cdot (-D\nabla c + c\mathbf{u})$
cellPe	S	Cell Peclet number	$\left\|\frac{\mathbf{u}h}{D_m}\right\|$
Dts	S	Time-scaling coefficient	δ_{ts}
udl	S	Dimensionless velocity	u_{dl}
D	S	Diffusion coefficient	D
R	S	Reaction rate	R
u, v, w	S	Velocity of c	u_i
N	B	Inward flux	N_0
c0	B	Concentration	c_0
Dm	S	Mean diffusion coefficient	$\frac{\sum_{i,j} D_{ij}\beta_i\beta_j}{\lvert\beta\rvert}, \beta = \mathbf{u}$
res	S	Equation residual	$\nabla \cdot (-D\nabla c + c\mathbf{u}) - R$

TABLE 2-33: APPLICATION MODE VARIABLES, CONVECTION AND DIFFUSION

NAME	TYPE	DESCRIPTION	EXPRESSION
res_sc	S	Shock capturing residual	$\nabla \cdot (c\mathbf{u}) - R$
da	S	Total time-scale factor	δ_{ts}

DIFFUSION

APPLICATION MODE NAME
chdi

TABLE 2-34: DEPENDENT VARIABLES, DIFFUSION

NAME	DESCRIPTION
c	Concentration

The application mode variables are:

TABLE 2-35: APPLICATION MODE VARIABLES, DIFFUSION

NAME	TYPE	DESCRIPTION	EXPRESSION
grad	S	Concentration gradient	∇c
dflux	S (V)	Diffusive flux	$-D\nabla c$
ndflux	B	Normal diffusive flux	$\mathbf{n} \cdot (-D\nabla c)$
Dts	S	Time scaling coefficient	δ_{ts}
D, Dx*i*x*j*	S	Diffusion coefficient	D
R	S	Reaction rate	R
N	B	Inward diffusive flux	N_0
kc	B	Mass transfer coefficient	k_c
cb	B	Bulk concentration	c_b
c0	B	Concentration	c_0

MAXWELL-STEFAN CONVECTION AND DIFFUSION

APPLICATION MODE NAME
chms

TABLE 2-36: DEPENDENT VARIABLES, MAXWELL-STEFAN CONVECTION AND DIFFUSION

NAME	DESCRIPTION
$\omega_1, \omega_2, \ldots, \omega_n$	Mass fractions

The application mode variables are:

TABLE 2-37: APPLICATION MODE VARIABLES, MAXWELL-STEFAN CONVECTION AND DIFFUSION

NAME	TYPE	DESCRIPTION	EXPRESSION
grad	S	Mass fraction gradient	$\nabla\omega$
dflux	S (V)	Diffusive flux	$-\rho\omega_k\sum_{l=1}^{n}\tilde{D}_{kl}\left(\nabla x_l+(x_l-\omega_l)\frac{\nabla p}{p}\right)+D^T\frac{\nabla T}{T}$
cflux	S (V)	Convective flux	$\rho\omega\mathbf{u}$
tflux	S (V)	Total flux	$\rho\omega_k\mathbf{u}-\rho\omega_k\sum_{l=1}^{n}\tilde{D}_{kl}\left(\nabla x_l+(x_l-\omega_l)\frac{\nabla p}{p}\right)+D^T\frac{\nabla T}{T}$
ndflux	B	Normal diffusive flux	$\mathbf{n}\cdot\left(-\rho\omega_k\sum_{l=1}^{n}\tilde{D}_{kl}\left(\nabla x_l+(x_l-\omega_l)\frac{\nabla p}{p}\right)+D^T\frac{\nabla T}{T}\right)$
ncflux	B	Normal convective flux	$\mathbf{n}\cdot\rho\omega\mathbf{u}$
ntflux	B	Normal total flux	$\mathbf{n}\cdot\left(\rho\omega_k\mathbf{u}-\rho\omega_k\sum_{l=1}^{n}\tilde{D}_{kl}\left(\nabla x_l+(x_l-\omega_l)\frac{\nabla p}{p}\right)+D^T\frac{\nabla T}{T}\right)$
x	S	Mole fraction	$\sum_{k=1}^{n}\omega_k/M_k$
M_mc	S	Total mole mass	$\sum_{k=1}^{n}M_k x_k$

TABLE 2-37: APPLICATION MODE VARIABLES, MAXWELL-STEFAN CONVECTION AND DIFFUSION

NAME	TYPE	DESCRIPTION	EXPRESSION
R	S	Reaction rate	R
DiT	S	Multicomponent thermal diffusion coefficient	D^T
M	S	Molecular weight	M
Dw*k*w*l*	S	Maxwell-Stefan diffusion coefficient	D_{kl}
Dts	S	Time scaling coefficient	δ_{ts}
udl	S	Dimensionless velocity	u_{dl}
rho	S	Density	ρ
T	S	Temperature	T
u, v, w	S	Velocity	$\mathbf{u}$
N	B	Inward mass flux	n_0
w0	B	Mass fraction	ω_0

The multicomponent diffusivities are constructed according to the number of species, their expressions are listed in Table 2-38. For two and three components, the multicomponent diffusivities are based on reference Ref. 1. For four components or

more, the multicomponent diffusivities are obtained numerically through matrix inversion.

TABLE 2-38: MAXWELL-STEFAN DIFFUSION AND CONVECTION—MULTICOMPONENT DIFFUSIVITIES

LABEL	TYPE	DESCRIPTION	EXPRESSION
DEw*k*w*l*	S	Two-component diffusivity	$\tilde{D}_{11} = \frac{\omega_2^2}{x_1 x_2} D_{12}$ $\tilde{D}_{12} = \tilde{D}_{21} = -\frac{\omega_1 \omega_2}{x_1 x_2} D_{12}$ $\tilde{D}_{22} = \frac{\omega_1^2}{x_1 x_2} D_{12}$

TABLE 2-38: MAXWELL-STEFAN DIFFUSION AND CONVECTION—MULTICOMPONENT DIFFUSIVITIES

LABEL	TYPE	DESCRIPTION	EXPRESSION
DEw*k*w*l*	S	Three-component diffusivity. Additional entries are constructed by cyclic permutation of the indices	$\tilde{D}_{11} = \dfrac{\dfrac{(\omega_2+\omega_3)^2}{x_1 D_{23}} + \dfrac{\omega_2^2}{x_2 D_{13}} + \dfrac{\omega_3^2}{x_3 D_{12}}}{\dfrac{x_1}{D_{12}D_{13}} + \dfrac{x_2}{D_{12}D_{23}} + \dfrac{x_3}{D_{13}D_{23}}}$ $\tilde{D}_{12} = -\dfrac{\dfrac{\omega_1(\omega_2+\omega_3)}{x_1 D_{23}} + \dfrac{\omega_2(\omega_1+\omega_3)}{x_2 D_{13}} - \dfrac{\omega_3^2}{x_3 D_{12}}}{\dfrac{x_1}{D_{12}D_{13}} + \dfrac{x_2}{D_{12}D_{23}} + \dfrac{x_3}{D_{13}D_{23}}}$ $\tilde{D}_{kj} = \tilde{D}_{jk}$
DEw*k*w*l*	S	n-component diffusivity, where $n \geq 4$	$\tilde{D}_{kl} = \tilde{D}_{lk} = N_{kl} - g$ $N_{kl} = (M^{-1})_{kl}$ $M_{kl} = \dfrac{\omega_k \omega_l}{g} - \tilde{C}_{kl}$ $\tilde{C}_{kl} = \begin{cases} \dfrac{x_k x_l}{D_{kl}} & k \neq l \\ -\displaystyle\sum_{m \neq k} \tilde{C}_{km} & k = l \end{cases}$ where $k \leq l \leq n$ and $g = \displaystyle\sum_{i=1}^{n-1} \left(\sum_{j=i+1}^{n} D_{ij} \right)$

ELECTROKINETIC FLOW

APPLICATION MODE NAME
chekf

TABLE 2-39: DEPENDENT VARIABLES, ELECTROKINETIC FLOW

NAME	DESCRIPTION
c	Concentration

The application mode variables are:

TABLE 2-40: APPLICATION MODE VARIABLES, ELECTROKINETIC FLOW

NAME	TYPE	DESCRIPTION	EXPRESSION
grad	S	Concentration gradient	∇c
dflux	S (V)	Diffusive flux	$-D\nabla c$
cflux	S (V)	Convective flux	$c\mathbf{u}$
mflux	S (V)	Electrophoretic flux	$-zu_m Fc\nabla V$
tflux	S (V)	Total flux	$-D\nabla c - zu_m Fc\nabla V + c\mathbf{u}$
ndflux	B	Normal diffusive flux	$\mathbf{n}\cdot(-D\nabla c)$
ncflux	B	Normal convective flux	$\mathbf{n}\cdot c\mathbf{u}$
nmflux	B	Normal electrophoretic flux	$\mathbf{n}\cdot(-zu_m Fc\nabla V)$
ntflux	B	Normal total flux	$\mathbf{n}\cdot(-D\nabla c - zu_m Fc\nabla V + c\mathbf{u})$
cellPe	S	Cell Peclet number	$\left\lvert\frac{(\mathbf{u} - zu_m F\nabla V)h}{D_m}\right\rvert$
Dts	S	Time-scaling coefficient	δ_{ts}
udl	S	Dimensionless velocity	u_{dl}
D	S	Diffusion coefficient	D
R	S	Reaction rate	R
um	S	Mobility	u_m
z	S	Charge number	z
u, v, w	S	Velocity	$\mathbf{u}$
V	S	Potential	V
N	B	Inward flux	N_0
c0	B	Concentration	c_0

TABLE 2-40: APPLICATION MODE VARIABLES, ELECTROKINETIC FLOW

NAME	TYPE	DESCRIPTION	EXPRESSION
gradpot	S	Potential gradient	∇V
Dm	S	Mean diffusion coefficient	$\frac{\sum_{i,j} D_{ij}\beta_i\beta_j}{\lvert\beta\rvert}$, $\beta = \mathbf{u} - zu_m F\nabla V$
res	S	Equation residual	$\nabla\cdot(-D\nabla c - zu_m Fc\nabla V + c\mathbf{u}) - R$
res_sc	S	Shock capturing residual	$\nabla\cdot(c\mathbf{u} - zu_m Fc\nabla V) - R$
da	S	Total time scale factor	δ_{ts}

NERNST-PLANCK

APPLICATION MODE NAME
chnp

TABLE 2-41: DEPENDENT VARIABLES, NERNST-PLANCK

NAME	DESCRIPTION
V	Electric potential
c1, c2,..., cn	Concentration

The application mode variables are:

TABLE 2-42: APPLICATION MODE VARIABLES, NERNST-PLANCK

NAME	TYPE	DESCRIPTION	EXPRESSION
c1	S	Concentration c1	$c_1 = -\frac{1}{z_1}\sum_{k=2}^{n} z_k c_k$
ci	S	Concentration ci (i = 2...n)	c_i
grad	S	Concentration gradient	∇c_k
dflux	S	Diffusive flux	$D\nabla c_k$
cflux	S	Convective flux	$c_k\mathbf{u}$
mflux	S	Electrophoretic flux	$zu_m Fc_k\nabla V$
tflux	S	Total flux	$-D\nabla c_k - zu_m Fc_k\nabla V + c_k\mathbf{u}$

TABLE 2-42: APPLICATION MODE VARIABLES, NERNST-PLANCK

NAME	TYPE	DESCRIPTION	EXPRESSION
J	S	Current density	$\sum_{k=1}^{n} Fz_k(-D_k\nabla c_k - z_k u_{mk} F c_k \nabla V)$
kappa	S	Ionic conductivity	$F^2 \sum_{i=1}^{n} z_i^2 c_i u_{mi}$
ndflux	B	Normal diffusive flux	$\mathbf{n} \cdot (-D\nabla c_k)$
ncflux	B	Normal convective flux	$\mathbf{n} \cdot c_k \mathbf{u}$
nmflux	B	Normal electrophoretic flux	$\mathbf{n} \cdot (-z u_m F c_k \nabla V)$
ntflux	B	Normal total flux	$\mathbf{n} \cdot (-D\nabla c_k - z u_m F c_k \nabla V + c_k \mathbf{u})$
nJ	B	Normal current density	$-\mathbf{n} \cdot \sum_{k=1}^{n} Fz_k(D\nabla c_k + z_k u_{mk} F c_k \nabla V)$
cellPe	S	Cell Peclet number	$\left\lvert \frac{(\mathbf{u} - z u_m F \nabla V)h}{D_m} \right\rvert$
Dts	S	Time-scaling coefficient	δ_{ts}
udl	S	Dimensionless velocity	u_{dl}
D	S	Diffusion coefficient	D
R	S	Reaction rate	R
um	S	Mobility	u_m
z	S	Charge number	z
u, v, w	S	Velocity	$\mathbf{u}$
V	S	Potential	V
gradV	S	Potential gradient	$\lvert\nabla V\rvert$
N	B	Inward flux	N_0
c0	B	Concentration	c_0
beta	S	Convective field	$\mathbf{u} - z u_m F c \nabla V$

TABLE 2-42: APPLICATION MODE VARIABLES, NERNST-PLANCK

NAME	TYPE	DESCRIPTION	EXPRESSION
Dm	S	Mean diffusion coefficient	$\frac{\sum_{i,j} D_{ij}\beta_i\beta_j}{\lvert\beta\rvert}$, $\beta = \mathbf{u} - zu_m F\nabla V$
res	S	Equation residual	$\nabla \cdot (-D\nabla c - zu_m Fc\nabla V + c\mathbf{u}) - R$
res_sc	S	Shock capturing residual	$\nabla \cdot (c\mathbf{u} - zu_m Fc\nabla V) - R$
da	S	Total time-scale factor	δ_{ts}

NERNST-PLANCK WITHOUT ELECTRONEUTRALITY

The implementation is exactly the same as the Electrokinetic Flow application mode; see page 35 of this manual.

Reference

1. C.F. Curtiss and R.B. Bird, "Multicomponent Diffusion," *Ind. Eng. Chem. Res.*, vol. 38, pp. 2515–2522, 1999.

Log-Formulation of the Turbulence Equations

The implementation in COMSOL Multiphysics of the k-ε and k-ω turbulence models are based on a logarithmic formulation of the equations. This chapter describes the formulation of the equations.

Logarithmic Formulation of the k-ε Turbulence Model

COMSOL has chosen to implement the logarithmic formulation of the k-ε equations as suggested by Ignat and others (Ref. 1). The equations assuming transient and non-isothermal flow are

$$\rho\frac{\partial \mathbf{U}}{\partial t} + \rho\mathbf{U}\cdot\nabla\mathbf{U} = \nabla\cdot\left[-P\mathbf{I} + (\eta + \eta_T)\left(\nabla\mathbf{U} + (\nabla\mathbf{U})^T - \frac{2}{3}\mathbf{I}(\nabla\cdot\mathbf{U})\right)\right] + \mathbf{F}$$

$$\frac{\partial \rho}{\partial t} + \nabla\cdot(\rho\mathbf{U}) = 0$$

$$\rho\frac{\partial \log k}{\partial t} + \rho\mathbf{U}\cdot\nabla k = \nabla\cdot\left[\left(\eta + \frac{\eta_T}{\sigma_k}\right)\nabla\log k\right] + \left(\eta + \frac{\eta_T}{\sigma_k}\right)(\nabla\log k)^2 +$$

$$\eta_T e^{-\log k}P(\mathbf{U}) - \frac{2}{3}\rho\nabla\cdot\mathbf{U} - \rho e^{(\log\varepsilon - \log k)}$$

$$\rho\frac{\partial \log\varepsilon}{\partial t} + \rho\mathbf{U}\cdot\nabla\log\varepsilon = \nabla\cdot\left[\left(\eta + \frac{\eta_T}{\sigma_\varepsilon}\right)\nabla\log\varepsilon\right] + \left(\eta + \frac{\eta_T}{\sigma_\varepsilon}\right)(\nabla\log\varepsilon)^2 +$$

$$C_{\varepsilon 1}\left[\eta_T e^{-\log k}P(\mathbf{U}) - \frac{2}{3}\rho\nabla\cdot\mathbf{U}\right] - \rho C_{\varepsilon 2}e^{(\log\varepsilon - \log k)}$$

where $P(\mathbf{u})$ is defined as

$$P(\mathbf{u}) = \frac{1}{2}(\nabla\mathbf{u} + (\nabla\mathbf{u})^T)^2 - \frac{2}{3}(\nabla\cdot\mathbf{u})^2$$

and η_T is the turbulent viscosity, defined as

$$\eta_T = \rho C_\mu e^{(2\log k - \log\varepsilon)}$$

Logarithmic Formulation of the k-ω Turbulence Model

The equations for the k-ω turbulence model, assuming transient and non-isothermal flow, are

$$\rho\frac{\partial \log k}{\partial t} + \rho\mathbf{U}\cdot\nabla k = \nabla\cdot[(\eta + \sigma_k\eta_T)\nabla\log k] + (\eta + \sigma_k\eta_T)(\nabla\log k)^2 + \eta_T e^{-\log k}P(\mathbf{U}) - \frac{2}{3}\rho\nabla\cdot\mathbf{U} - \beta_k\rho e^{\log\omega}$$

$$\rho\frac{\partial \log \omega}{\partial t} + \rho\mathbf{U}\cdot\nabla\log\omega = \nabla\cdot[(\eta + \sigma_\omega\eta_T)\nabla\log\omega] + (\eta + \sigma_\omega\eta_T)(\nabla\log\omega)^2 + \alpha\left[\eta_T e^{-\log k}P(\mathbf{U}) - \frac{2}{3}\rho\nabla\cdot\mathbf{U}\right] - \rho\beta e^{\log\omega}$$

where $P(\mathbf{u})$ is defined as

$$P(\mathbf{u}) = \frac{1}{2}(\nabla\mathbf{u} + (\nabla\mathbf{u})^T)^2 - \frac{2}{3}(\nabla\cdot\mathbf{u})^2$$

and η_T is the turbulent viscosity, defined as

$$\eta_T = \rho e^{\log k - \log\omega}$$

Reference

1. L. Ignat, D. Pelletier, and F. Ilinca, "A universal formulation of two-equation models for adaptive computation of turbulent flows," *Computer methods in applied mechanics and engineering*, vol. 189, pp. 1119–1139, 2000.

Special Element Types For Fluid Flow

The list of predefined elements in the Incompressible Navier-Stokes application mode and its variants includes some special element types in addition to the standard Lagrange elements. These elements are potentially useful for applications in fluid dynamics and are listed in Ref. 1.

All these elements include bubble shape functions to approximate the velocity variables and/or discontinuous shape functions for approximating pressure. The table below provides a short description of these special elements.

TABLE 2-43: INCOMPRESSIBLE NAVIER-STOKES—SPECIAL ELEMENT TYPE

ELEMENT NAME	2D	3D	DESCRIPTION
$P_1+ P_1$ (Mini)	√	√	Similar to the Lagrange - Linear element with an additional bubble shape function to approximate the velocity variables
$P_2 P_0$	√		The pressure is approximated by a discontinuous function which is piecewise constant (that is, of order 0) in each element and discontinuous on the element edges
$P_2+ P_1$	√		Similar to Lagrange - $P_2 P_1$ with an additional bubble shape function to approximate the velocity variables. Considered to be a good element (Ref. 1)
$P_2 (P_1+P_0)$	√	√	Similar to Lagrange - $P_2 P_1$ with an additional discontinuous shape function to approximate the pressure
$P_2 P_{-1}$	√		Similar to Lagrange - $P_2 P_1$ with the exception that the pressure is described by a linear shape function which is discontinuous at the element edges. This element is pointwise divergence-free
$P_2+ P_{-1}$ (Crouzeix-Raviart)	√	√	Similar to Lagrange - $P_2 P_1$ with an additional bubble shape function to approximate the velocity variables and a linear shape function that is discontinuous on the element edges to approximate the pressure. Considered to be a good element (Ref. 1)

The notation used for the element names is taken from Ref. 1 and summarized below:

- $P_m P_n$, where $m > 0$ and $n > 0$, denotes that the velocity variables are approximated by a polynomial shape function of order m and that the pressure is approximated by

a polynomial shape function of order n. Both the velocity and the pressure variables are continuous on the element edges.

- $P_m^+ P_n$ is similar to the above with a bubble shape function added to approximate the velocity variables. The bubble shape function is of order 3 in 2D (order 4 in 3D) and is zero on the element edges.
- $P_m P_{-n}$, where $m > 0$ and $n \geq 0$, is similar to the first case ($P_m P_n$) with the exception that the shape function for the pressure is discontinuous on the element edges.
- $P_m (P_n + P_q)$ is also similar to the first case ($P_m P_n$) with an additional shape function added to approximate the pressure.

It is difficult to choose the optimal element for a specific model. The table above provides some brief characteristics on each element. Ref. 1 is recommended for further reading on these elements.

Exploring element-specific variables Some of the predefined elements introduce additional variables. For the elements that include a bubble shape function, the velocity is approximated by:

$$u = \mathrm{ul} + \mathrm{ub} \tag{2-2}$$

$$v = \mathrm{vl} + \mathrm{vb} \tag{2-3}$$

$$w = \mathrm{wl} + \mathrm{wb} \tag{2-4}$$

where ul, vl, and wl are contributions from the Lagrange shape functions, and ub, vb, and wb are contributions from the bubble shape functions. Each contribution can be plotted separately. For example, to plot the contribution from the bubble shape function to the velocity when using the Navier-Stokes application mode, plot the expression `ub_chns`.

Similarly, for the $P_2 (P_1 + P_0)$ element, the pressure is represented by:

$$p = p_1 + p_2 \tag{2-5}$$

You can plot each pressure contribution separately by using the expressions `p1_chns` and `p2_chns`, respectively, in the Incompressible Navier-Stokes application mode.

Values for integration and constraint order Each predefined element type has its own default values for **integration order** (**gporder**) and **constraint order** (**cporder**). For the bubble shape functions, the required integration order is relatively high. These elements in combination with a large and dense mesh can therefore lead to high

memory consumption. For this reason, the default **gporder** value for the Crouzeix-Raviart element ($P_2 + P_{-1}$) in 3D is somewhat lower than what would be theoretically required. For the other element types that include bubble shape functions, you may have to reduce **gporder** manually by one or two units to reduce memory consumption.

Reference

1. P.M. Gresho and R.L. Sani, *Incompressible Flow and the Finite Element Method*, 2nd vol., John Wiley & Sons Ltd, 2000.

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