

1 Features Added in Virtual Reactor 5.4

1.1 Implementation of Full Navier-Stokes Flow Model

Generally, the gas mixture flow in the growth chamber is described by the following set of equations:

Continuity:

$$\nabla \cdot (\rho \vec{V}) = 0 \quad (1)$$

Momentum:

$$\nabla \cdot (\rho \vec{V} \vec{V}) = -\nabla p_d + \rho \vec{g} + 2 \text{Div}(\mu \dot{S}) - \frac{2}{3} \nabla(\mu \nabla \cdot \vec{V}) \quad (2)$$

Species transport:

$$\nabla \cdot (\rho \vec{V} c_i + \vec{J}_i) = \dot{w}_i, \quad i = 1, \dots, N_s \quad (3)$$

Energy:

$$\nabla \cdot (\rho \vec{v} h + \vec{q}) = 0 \quad (4)$$

Equation of state:

$$p_t = \rho RT \sum_{i=1}^{N_s} \frac{c_i}{M_i}, \quad i = 1, \dots, N_s, \quad (5)$$

Two models of flow dynamics are implemented in **Virtual Reactor 5.4**, namely, full Navier-Stokes model and model of hypersonic flow. In the earlier versions of Virtual Reactor, the latter model was only available.

The total pressure p_t is considered as the sum of two components, static (reference) pressure p_{st} , which is constant throughout the whole flow domain, and dynamic pressure p_d whose drop is considered as the driving force for the flow.

The model of hypersonic flow assumes $p_d \ll p_{st}$, so that

$$p_t \approx p_{st} \quad (6)$$

Within this model, the pressure drop inside the domain is only accounted for in the momentum equation via the dynamic pressure gradient, while the static pressure is used in the equation of state and in the determination of the partial pressures of the gas mixture species:

$$p_{st} = \rho RT \sum_{i=1}^{N_s} \frac{c_i}{M_i} \quad (7)$$

$$p_i = c_i \frac{M}{M_i} p_{st}, \quad i = 1, \dots, N_s \quad (8)$$

This assumption is valid in modeling low Mach number flows in gas domains, failing, in particular, in case of flow in complex systems involving considerable hydraulic resistance, like

- Flow in porous media
- Flow in gas domains consisted of several zones connected via narrow channels.

So this assumption may fail to treat the flow in SiC powder charge (especially in case of small granule diameter and low porosity) and the flow in growth domains involving several zones separated by slits, porous materials, etc.

The full Navier-Stokes model implemented in **Virtual Reactor 5.4** assumes

$$p_t = p_{st} + p_d \quad (9)$$

$$p_t = \rho RT \sum_{i=1}^{N_s} \frac{c_i}{M_i} \quad (10)$$

$$p_i = c_i \frac{M}{M_i} p_t, \quad i = 1, \dots, N_s \quad (11)$$

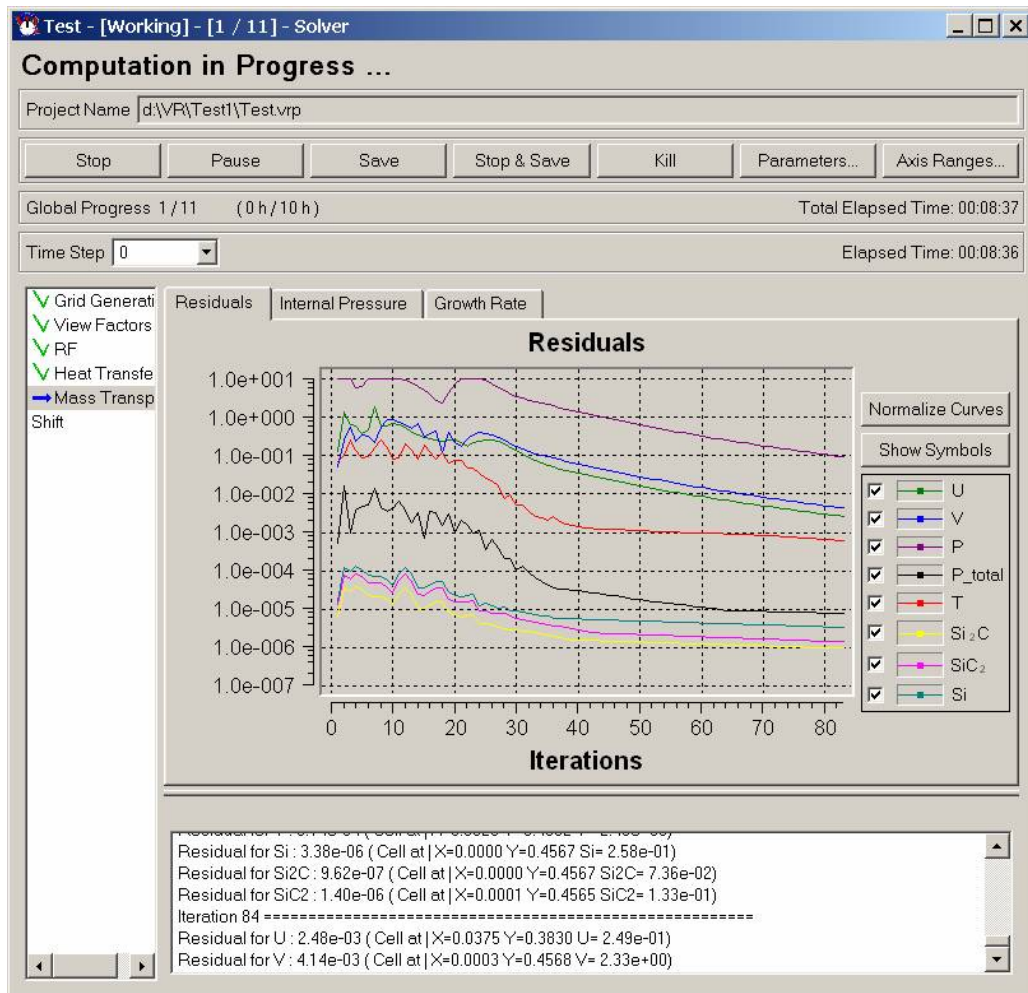
This model accounts the effect of the pressure drop inside the growth domain on all chemical processes in the growth system.

1.2 Extension of Output Information

Additional diagnostics about the species transport was added into the computation log file. The following quantities are reported:

- Integral mass fluxes on boundaries of the growth chamber (in kg):
 - ✓ Total mass flux
 - ✓ Chemical fluxes for each species (on all catalytic boundaries)
 - ✓ Filtration fluxes for each species (on porous walls and thin slits)
 - ✓ Sum Fluxes for each species (sum of chemical and filtration fluxes)
- Average growth rate for each boundary (on all catalytic boundaries). Positive value corresponds to growth/deposition, negative – to sublimation/etching
- Mass of all blocks at the current time step (in kg)

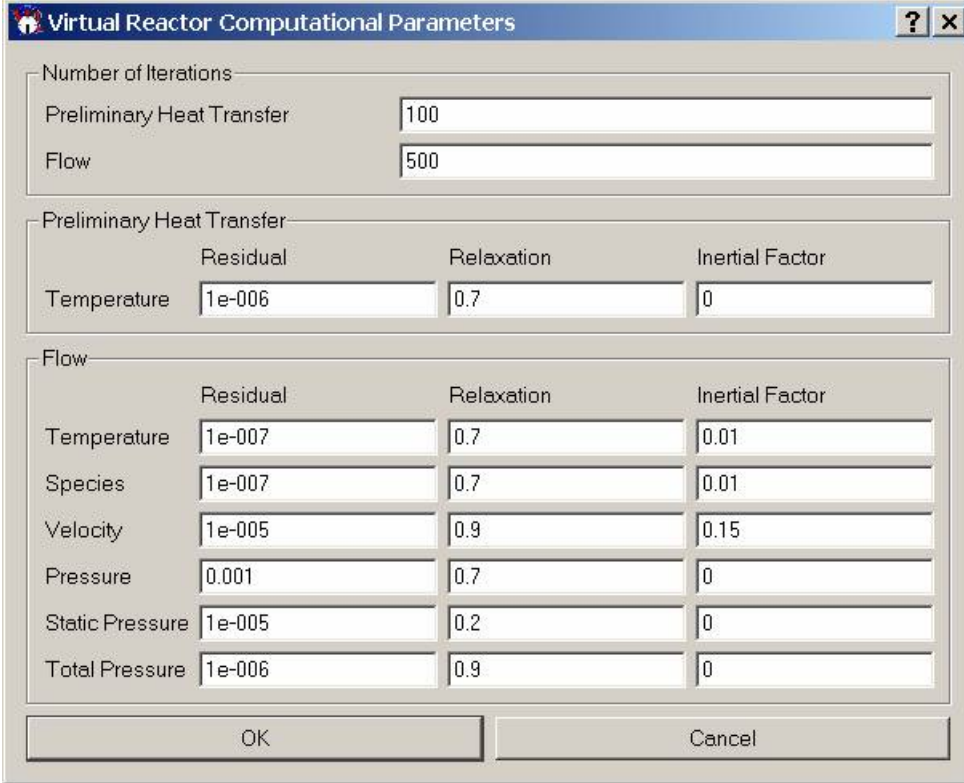
1.3 Changes in Solution Monitor



The following options were added to the solution monitor:

1.3.1 Runtime modification of the computational parameters

The computational parameters (number of iterations, threshold residuals, relaxation and inertial factors) set before starting the computation can now be changed during the computation run using the **Computational Parameters** dialog that can be opened by the user with **Parameters** button.



| Virtual Reactor Computational Parameters | | | |
|--|----------|------------|-----------------|
| Number of Iterations | | | |
| Preliminary Heat Transfer | 100 | | |
| Flow | 500 | | |
| Preliminary Heat Transfer | | | |
| | Residual | Relaxation | Inertial Factor |
| Temperature | 1e-006 | 0.7 | 0 |
| Flow | | | |
| | Residual | Relaxation | Inertial Factor |
| Temperature | 1e-007 | 0.7 | 0.01 |
| Species | 1e-007 | 0.7 | 0.01 |
| Velocity | 1e-005 | 0.9 | 0.15 |
| Pressure | 0.001 | 0.7 | 0 |
| Static Pressure | 1e-005 | 0.2 | 0 |
| Total Pressure | 1e-006 | 0.9 | 0 |
| OK | | Cancel | |

1.3.2 Specification of the Axis Ranges

Manual specification of ranges of axes in all plots in the Solution Monitor is available using the **Settings** dialog window that can be opened by the user with **Axis Ranges** button.

Each of the four ranges (X_{\min} , X_{\max} , Y_{\min} and Y_{\max}) can individually be set manually or calculated automatically. Note that if X-axis (iterations) ranges are manually assigned and Y-axis ranges are set to be found automatically, the Y-axis range are calculated accounting for the data within the X-axis range only. This provides an easy specification of pictorial visualization of convergence of parameters abruptly changing on the starting iterations and slowly varying during the further convergence.

Solution Monitor Settings

GHT Residuals

X Axis Min AutoDetect X Axis Max AutoDetect

Y Axis Min AutoDetect Y Axis Max AutoDetect

Maximum Temperature

X Axis Min AutoDetect X Axis Max AutoDetect

Y Axis Min AutoDetect Y Axis Max AutoDetect

Fitting Temperature

X Axis Min AutoDetect X Axis Max AutoDetect

Y Axis Min AutoDetect Y Axis Max AutoDetect

Fitting Power

X Axis Min AutoDetect X Axis Max AutoDetect

Y Axis Min AutoDetect Y Axis Max AutoDetect

MT Residuals

X Axis Min AutoDetect X Axis Max AutoDetect

Y Axis Min AutoDetect Y Axis Max AutoDetect

Axial Growth Rate

X Axis Min AutoDetect X Axis Max AutoDetect

Y Axis Min AutoDetect Y Axis Max AutoDetect

Internal Pressure

X Axis Min AutoDetect X Axis Max AutoDetect

Y Axis Min AutoDetect Y Axis Max AutoDetect

OK Cancel

1.3.3 Normalization of Residuals

Variation of the absolute and normalized residuals can be visualized using the **Normalize Curves** button. If it is pressed, the residuals are normalized with respect to their maximum value, so the maximum value of the normalized residuals is always equal to unity. This allows a pictorial visualization of relative drop of residuals whose absolute values differ considerably.

1.4 Changes in Specification of the Porous Wall Parameters

The option of automatic calculation of wall thickness in specification of *Porous Wall* and *Thin Slit* boundary conditions is made user defined. In the earlier versions, the wall thickness on internal boundaries was always calculated automatically from the adjacent solid block geometry, which imposed some restrictions on specification of the adjacent blocks. Now the user can always set the wall thickness explicitly.

1.5 Fixing Errors

Several found errors have been fixed.