CASE STUDY /

Ansys + American Boronite Corporation

"We have been able to use Ansys computational fluid dynamics (CFD) simulation software to model our unique chemical vapor deposition (CVD) systems to troubleshoot experiments and prototype new designs for producing and processing the synthesized nanomaterials. With their software packages we can optimize the configuration of our systems to increase production, efficiency and ensure consistent quality in our products."

William Livernois
Chemical Engineer / American Boronite Corporation

/ Introduction

As a manufacturer of boron nitride nanotubes, we must optimize efficiency at each stage of our continuous production system to scale up effectively. With Ansys computational fluid dynamics (CFD) software, we can simulate many different configurations of our process at the same time, thus saving time and money during process development. Our simulation results have also inspired new and improved designs that have led to significant development progress.

/ Company Description

At Boronite, we are developing and scaling a completely new technique for producing boron nitride nanotubes in continuous forms as either spun yarn or non-woven tape. We are the first in the world to develop such a process for continuous production on a commercial scale.

/ Challenges

Because the reactions within our CVD reactors are multiphase, simulation is critical for understanding the resultant heat and mass transfer. There are not only multiple sources of heat transfer (e.g., radiation and convection/conduction) that are complicated by interacting gas phases but also a variety of moving parts that interact with the materials and change the timing and velocities upstream.

/ Technology Used

- Ansys Mechanical™
- Ansys Fluent®

/ Engineering Solution

Most simulations were conducted using single phase compressible flow to make our initial calculations. We then compared temperature profiles from these simulations to known run data from the reactors. In some cases, the single phase, compressible buoyant flow was enough to determine potential temperature profiles and gradients in the reactor. In other cases, we used multiphase flow models (such as VOF or Eulerian models) or discrete phase models to get a better idea of the heat and mass transfer occurring in the reactor. We compared both transient and steady-state solvers to determine the behavior and stability of the setups throughout the process.

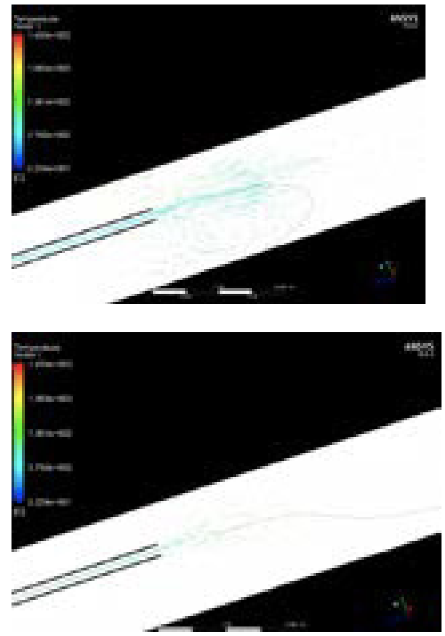

Figure 1. A cross section of a 3D single phase simulation used to determine eddy sizes and temperature gradients as a function of injection gas velocity.

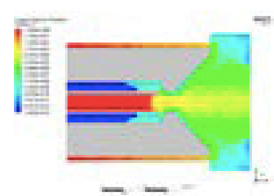

Figure 2. Two-phase mizer modeled using a 2D (axisymmetric) solver. A transient solver was used to determine fluid buildup over time.

Benefits

During the design process for new parts (e.g., injectors or post-processing manipulators), we could run concurrent simulations to find a correlation between the downstream properties and variables while validating the model with the setup. For instance, in our yarn spinning system, we varied gas flow rates, spinning rates and coupling distances before converging on a design. This eliminated many design iterations that otherwise would have been necessary. In addition, this debugging process also allows us to check for potentially dangerous configurations (usually caused by high temperature or pressure gradients), thus improving the safety of our workplace and the reliability of our process. We used Ansys post-processing software to display the data in a polished format for presentations and meetings.

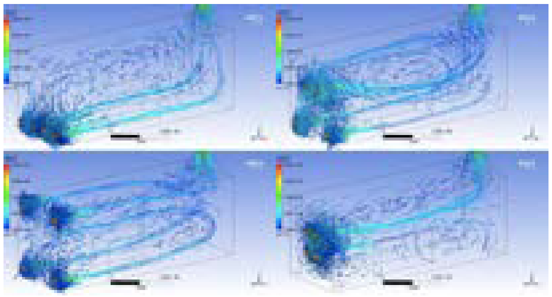

Figure 3. Comparison of enclosure setups (3D compressible flow) used to minimize stagnant zones, minimize backflow and improve venting.

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