COMPUTATIONAL FLUID DYNAMICS MODELING ANALYSIS OF COMBUSTORS

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INTRODUCTION:

In the current fiscal year FY01, several CFD simulations were conducted to investigate the effects of moisture in biomass/coal, particle injection locations, and flow parameters on carbon burnout and NO_x inside a 150 MW GEEZER industrial boiler. Various simulations were designed to predict the suitability of biomass cofiring in coal combustors, and to explore the possibility of using biomass as a reburning fuel to reduce NO_x. Some additional CFD simulations were also conducted on CERF combustor to examine the combustion characteristics of pulverized coal in enriched O_2/CO_2 environments. Most of the CFD models available in the literature treat particles to be point masses with uniform temperature inside the particles. This isothermal condition may not be suitable for larger biomass particles. To this end, a stand alone program was developed from the first principles to account for heat conduction from the surface of the particle to its center.

It is envisaged that the recently developed non-isothermal stand alone module will be integrated with the Fluent solver during next fiscal year to accurately predict the carbon burnout from larger biomass particles. Anisotropy in heat transfer in radial and axial will be explored using different conductivities in radial and axial directions. The above models will be validated/tested on various full-scale industrial boilers. The current NO_x modules will be modified to account for local CH, CH_2, and CH_3 radicals chemistry, currently it is based on global chemistry. It may also be worth exploring the effect of enriched O_2/CO_2 environment on carbon burnout and NO_x concentration..

Research Objectives:

The research objective of this study is to develop a 3-Dimensional Combustor Model for Biomass Co-firing and reburning applications using the Fluent Computational Fluid Dynamics **Code.**

Long Term Goals:

Development/Validation of specialized CFD sub-models for predicting unburned carbon and NO_x emissions from co-firing/reburning of biomass in pc full utility boilers. These sub-models can be used as a component in virtual demonstration of power plant. Also, NETL will develop an extensive CFD/experimental database for different coals. This project supports the mission of two product lines, viz., Vision 21 and Advanced Power Systems.

Summary of Accomplishments:

- Integrated moisture submodel with our recently developed CBK model
- Developed/tested a model to include the effect of moisture on coal/biomass combustion characteristics on full scale 150 MW GE-EER boiler
- Tested the robustness of integrated "moisture and CBK submodel" with extreme levels of moisture fractions in biomass to predict the flame lift-off in a pilot scale combustor
- It was inferred that the CFD simulations can be used to predict the burnout of different biomass particle sizes. It can assist in determining the optimum biomass size that can be successfully used in coal/biomass cofiring in industrial boilers

- Developed a model to incorporate conduction effects in radial and axial directions
- Created an animation to depict the particle orientation during its trajectory in a combustor
- Created an animation to show the effect of moisture on flame characteristics inside the CERF combustor
- Created an animation to show the flow characteristics inside an industrial boiler

Results:

The computer simulations of coal fired combustors are an economically efficient tool for evaluating the design and control strategies to improve energy (fuel) efficiency, process stability and emissions control. The current state-of-the-art technology is now capable of *solving* the complex interdependent processes like fluid flow, turbulence, particle trajectories, heat transfer, soot generation and heterogeneous and homogeneous chemical reactions involved in fossil fuel combustion. However, the complete description of the chemistry of devolatilization and char oxidation is still based on kinetically simple empirical models that do not account for the chemical structure and complicated physics of the process. A recent sensitivity study of a CFD-based coal combustion model has shown that uncertainty in the devolatilization/oxidation parameters has a dominant effect on unburned carbon in model predictions (Jones et al., 1999). The purpose of this study is to perform some exploratory simulations in a lab/pilot scale combustor which examines the effects of fuel shape, size and injection location on unburned carbon and NO_x emissions.

The mathematical model used here is based on the commercial CFD code, FLUENT, where the gas flow is described by the time averaged equations of global mass, momentum, enthalpy and species mass fractions. The particle-phase equations formulated in Lagrangian form, and the coupling between phases are introduced through particle sources in the Eulerian gas-phase equations. The standard k-ϵ turbulence model, two-mixture-fraction probability density function (PDF), and the Discrete Ordinate radiation models are used in the present simulations. The coal devolatilization is simulated using the two-competing-rates Kobayashi model, and the char oxidation is modeled as the kinetics controlled surface reaction. The biomass devolatilization is incorporated using an Arrhenius-type, first order kinetic rate model. The biomass char oxidation is controlled by diffusion-limited surface reaction, and it is modeled as a constant density process. The standard FLUENT code has been updated with the modified char oxidation sub-models for coal and biomass via an externally defined user function.

The Combustion and Environmental Research Facility (CERF) engineers at the National Energy Technology Laboratory (NETL,Pittsburgh, PA, USA) are working together with FLUENT to develop and validate comprehensive combustion sub-models for cofiring biomass in pulverized coal boiler. This fundamental research is focussed on developing strategies for NOx reductions by reburning highly volatile, moist biofuels in utility boilers. Minimizing the unburned carbon in ash is one of the factors used to evaluate biomass fuels for utility boilers. Accurate prediction of unburned carbon in a highly fluctuating environment, like that found in utility boilers, requires the use of advanced carbon burnout kinetic models in CFD simulations.

This study involved the development of FLUENT subroutines for biomass combustion/ cofiring using available experimental data and first principle mathematical models that provide accurate estimation of kinetic and CFD model parameters for devolatilization and diffusion-controlled char burnout. Two sets of drying functions have been developed to include the effect of moisture present on the surface of coal/ biomass, and embedded in the char, typical of that found in low rank coals.

The effect of moisture on the surface of the coal/biomass is incorporated using a droplet/ vaporization model in FLUENT. The evaporation of moisture embedded in char is included via a surface reaction in a novel way that accounts for char burnout due to steam gasification. Another key concern in developing an accurate model for biomass combustion is accounting for significant asphericity in biomass char particles, which plays a key role in char burnout. To this end, an enhancement factor that accounts for the large length/diameter aspect ratio in the burning of biomass particle has been explicitly derived for FLUENT computations.

In FY01, we examined a number of interesting exploratory CFD simulations related to the CERF pilot scale combustor geometry and a T-fired industrial boiler have been conducted to examine the effects of biomass particle size and residence time on carbon burnout. Interestingly, despite ten times larger biomass (switch grass) particle size relative to coal, blending biomass with coal in the boiler actually reduced the unburned carbon. This phenomenon can be attributed to the high volatile content of the switch grass. A few additional exploratory CFD simulations were performed on the CERF combustor to examine the effect of O_2/CO_2 environment on NOx emissions. From the preliminary results, a reduction of 39% in NO x (On lb/MBTU basis) was observed when compared with the combustion of coal in air.

Over the next year, it is expected that 3D CFD simulations will be conducted for at least three full -scale utility boilers to asses the design and operational issues. The validated 3D CFD model, in conjunction with the engineering guidelines for allowable biomass type, particle size, and moisture will also be related to biomass fuel handling and process economics work for various power plant equipment and burner design/injection schemes. This CFD modeling - with new biomass cofiring routines will represent a new capability for commercial software and should nicely complement goals related to the co-firing of opportunity fuels, and the longer-term need to couple and integrate 3D CFD simulations with plant-modeling software for dynamic simulations. Information from the full-scale demonstrations will also provide feedback for refinement of the CFD model and insight into design and operational issues that are important for planning future utility biomass cofiring demonstration projects.

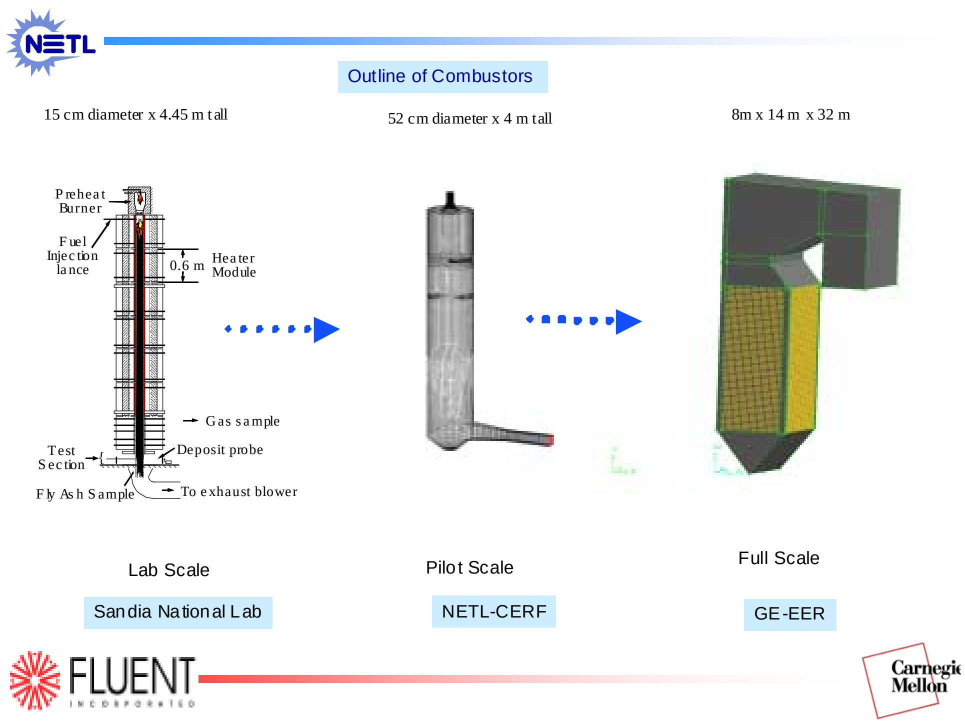
PUBLICATIONS

- Gera, D., Mathur, M., Freeman, M., O”Dowd, (2001), “Moisture and Char Reactivity Modeling in Pulverized Coal Combustors,” **<u>Combustion Science & Technology</u>**, ***Accepted for publication in Combustion Science and Technology.***
- Gera, D., Mathur, M., Freeman, M., O”Dowd, W.J., Walbert, G., Robinson, A., (2001), Computational Fluid Dynamics Modeling for Evaluating Design and Operational Issues for Biomass Cofiring in Coal-Fired Boilers,” 5th International Biomass Conference of the Americas, Orlando, FL, Sep 17-21
- Gera, D., Mathur, M., Freeman, M., O”Dowd, (2001), “Effect of Moisture and Variable Char Reactivity On Biomass/Coal Cofiring Units,” 2001 Joint AFRC/JFRC/IEA Combustion Symposium, Kauai, HI, Sep 9-12
- Gera, D., Mathur, M., Freeman, M., O”Dowd, (2001), “On the CFD Analysis of 500,000 Btu/Hr Combistor Using Enriched O_2 and Recycled Flue Gas,”2001 Joint AFRC/JFRC/IEA Combustion Symposium, Kauai, HI, Sep 9-12
- Gera, D., Mathur, M., Freeman, M., Walbert, G., Robinson, A., (2000), "Computational Fluid Dynamics Modeling For Biomass Cofiring Design In Pulverized Coal Boilers," Bioenergy'2000, Buffalo, NY, October 16-20, 2000
- Gera, D., Mathur, M., Freeman, M., (2001), “Moisture and Char Reactivity Modeling in Pulverized Coal Combustors,” Fluent’s Spring Newsletter

Future Recommendations:

- Incorporate non-isothermal treatment of the particle in Fluent Code
- Perform additional coal/biomass cofiring runs on various industrial boilers around WV and PA as requested by DOE
- Develop advanced NOx reburning modules to account for local CH, CH_2, and CH_3 radicals' chemistry
- Conduct full scale simulations for to examine the combustion characteristics of pulverized coal /biomass in enriched O_2/CO_2 environments
- Validate particle drying function with the available experimental data on an industrial boiler
- Participate in experimental measurements at CERF to measure NO_x and carbon burnout with different coal/biomass configurations.

Vision 21- Figures Photographs.



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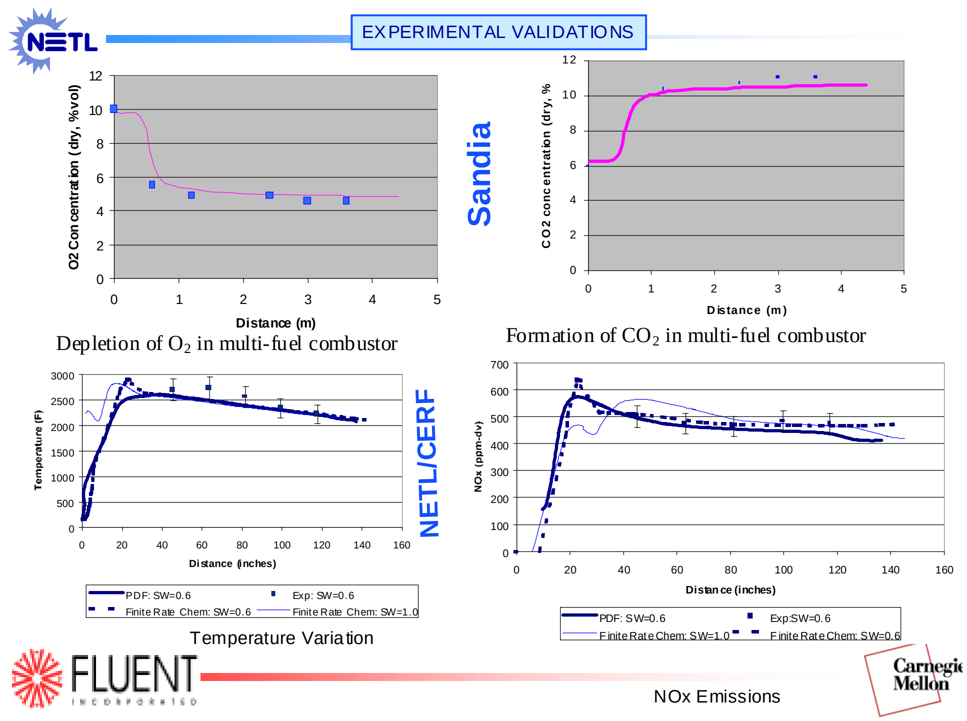
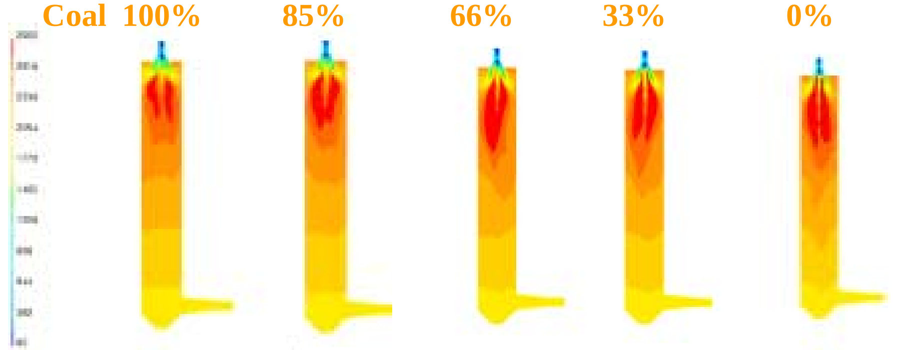


Vision 21- Figures Photographs.

Temperature Profiles

Coal 100% 85% 66% 33% 0%



0% 15% 33% 66% 100% SWG

NETL-CERF

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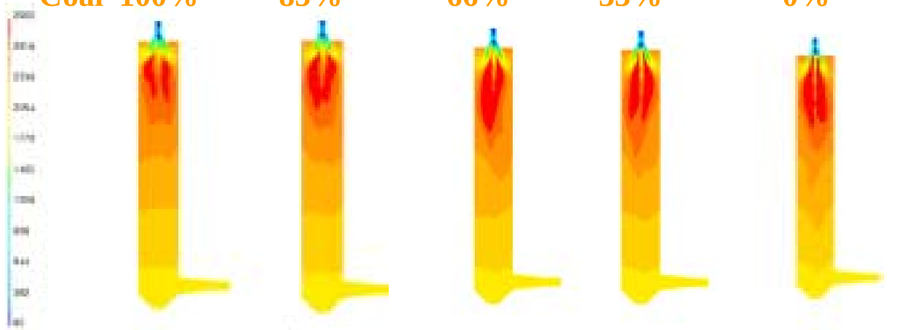
Temperature Profiles

Coal 100% 85% 66% 33% 0%



0% 15% 33% 66% 100% SWG

NETL-CERF

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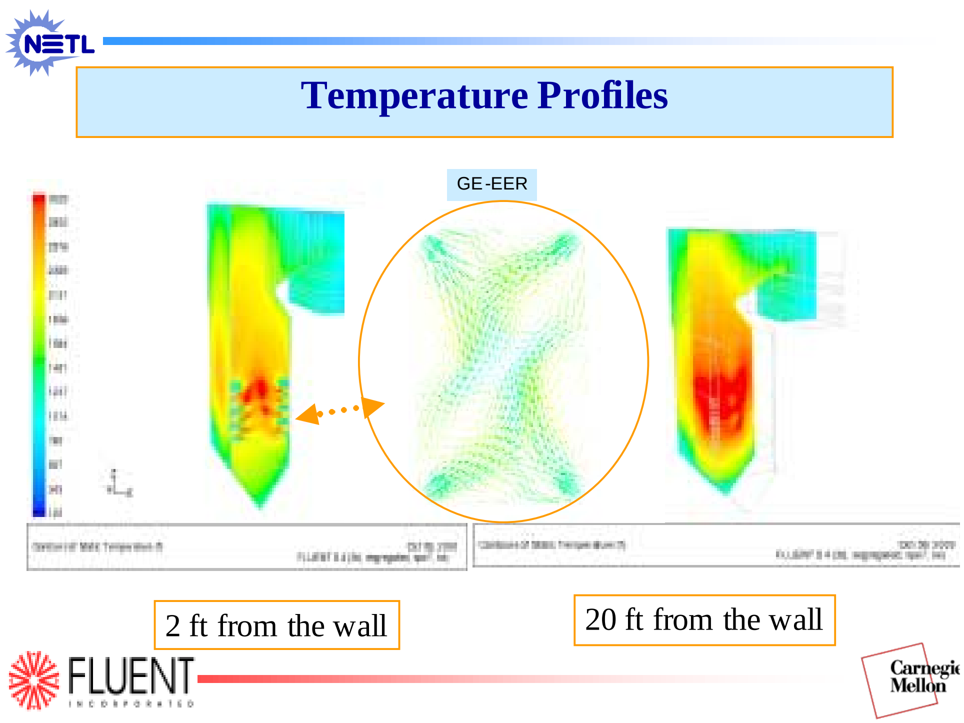

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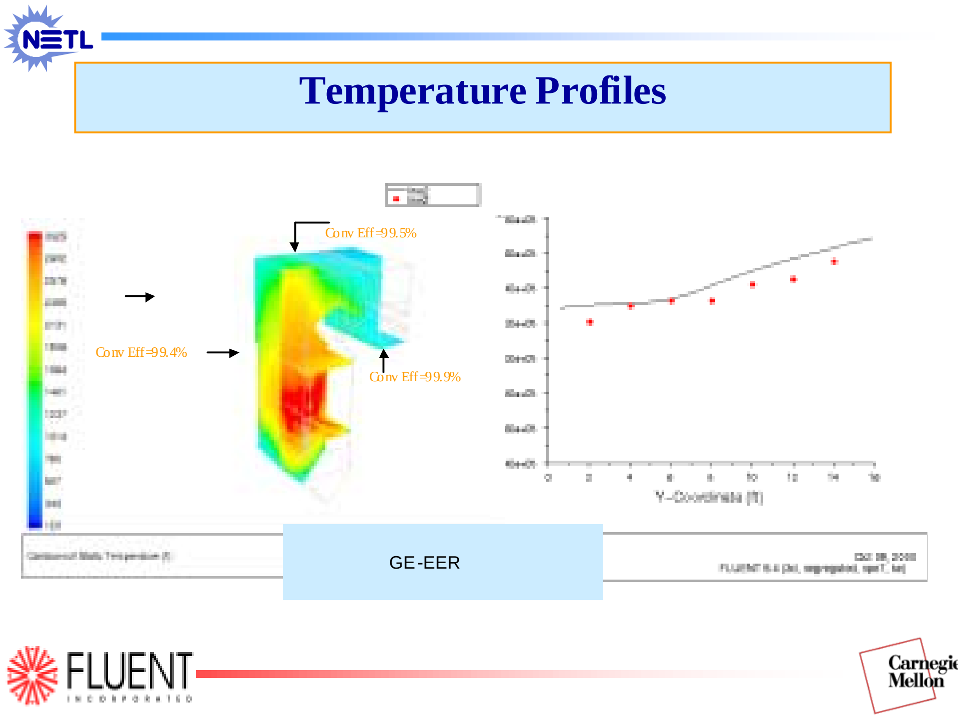

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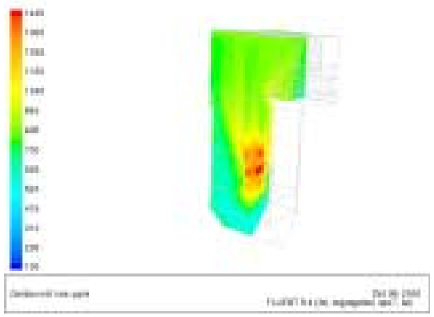
Contours of NOx Concentration (PPM)



Contours of O2 mole Fractions (%)

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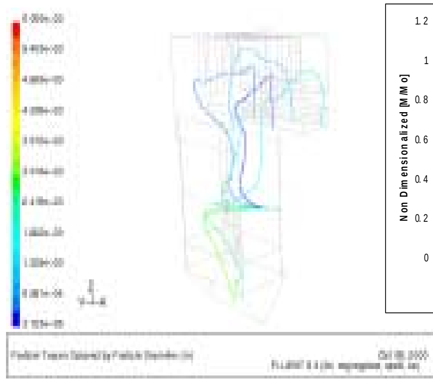
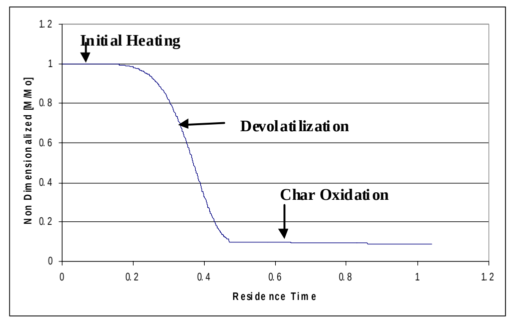
Typical Biomass Particle Burnout





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NETL

Table 1: Predicted and measured unburned carbon in SNL Multifuel Combustor (MFC)

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% SWG (Energy Basis)	Fuel Feed Rate (g/min)	Predicted Unburned Carbon Loss (Mass %)	**Measured Unburned Carbon Loss (Mass %)**	Predicted Carbon Percentage in Ash (%)	**Measured Carbon Percentage in Ash (%)**
100	44.4	2.3	**2.3**	19.9	*
66	36.6	2.3	**2.3**	19.6	**17.0**
33	25.5	2.6	**3.3**	22.9	**25.6**
15	22.4	3.8	**3.6**	32.1	**28.6**
0	19.6	4.8	**4.8**	37.8	**34.2**

Table 2: Combustion efficiency and residence times of various SWG particle sizes and pulverized coal in CERF 3-D CFD simulations

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Location in CERF Combustor – Distance from Burner	Comb. Eff (Res. Time) Pulverized (COAL)	Comb. Eff (Res.Time) 200 μm SWG	Comb. Eff (Res. Time) 400 μm SWG	Comb. Eff (Res. Time) 600 μm SWG	Comb. Eff (Res. Time) 800 μm SWG	Comb. Eff (Res. Time) 1 mm SWG
45"	95.4 (1.12 s)	97.7 (0.57 s)	95.3 (0.16 s)	46.5 (0.11 s)	3.25 (0.10 s)	2.16 (0.10 s)
99"	99.7 (2.55 s)	100.0 (1.67 s)	100.0 (0.84 s)	95.3 (0.39 s)	94.2 (0.24 s)	45.5 (0.22 s)
Convective Section	99.7 (3.1 s)	100.0 (2.13 s)	100.0 (1.37 s)	*	*	*

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